

10/516884

=> file registry

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STRUCTURE FILE UPDATES: 6 DEC 2007 HIGHEST RN 957014-20-9
DICTIONARY FILE UPDATES: 6 DEC 2007 HIGHEST RN 957014-20-9

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TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

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<http://www.cas.org/support/stngen/stndoc/properties.html>

=> file zcaplus

FILE 'ZCAPLUS' ENTERED AT 10:07:24 ON 07 DEC 2007
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FILE COVERS 1907 - 7 Dec 2007 VOL 147 ISS 25
FILE LAST UPDATED: 6 Dec 2007 (20071206/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate
substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'ZCAPLUS' FILE

=> d stat que L72

L70	362	SEA	FILE=ZCAPLUS	ABB=ON	PLU=ON	TAKAKI K?/AU
L71	929	SEA	FILE=ZCAPLUS	ABB=ON	PLU=ON	YAMASAKI Y?/AU
L72	7	SEA	FILE=ZCAPLUS	ABB=ON	PLU=ON	L70 AND L71

=> d stat que L73

10/516884

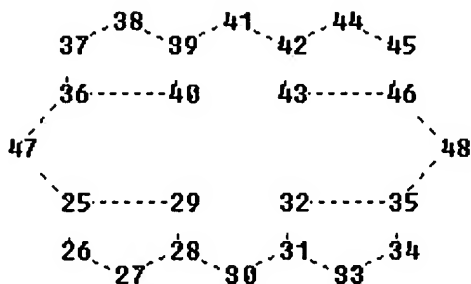
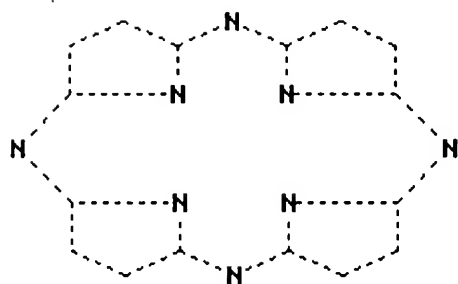
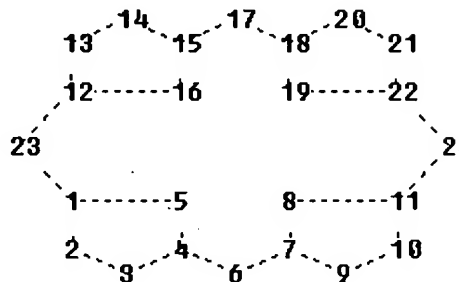
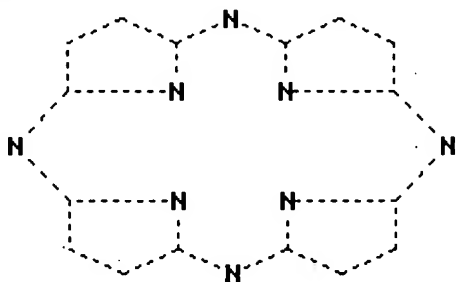
L4

STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:

Uploading L4b.str



ring nodes :

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23
24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44		
45	46	47	48																			

ring bonds :

1-2	1-5	1-23	2-3	3-4	4-5	4-6	6-7	7-8	7-9	8-11	9-10	10-11	11-24	12-13
12-16	12-23	13-14	14-15	15-16	15-17	17-18	18-19	18-20	19-22	20-21	21-22			
22-24	25-26													
25-29	25-47	26-27	27-28	28-29	28-30	30-31	31-32	31-33	32-35	33-34	34-35			
35-48	36-37													
36-40	36-47	37-38	38-39	39-40	39-41	41-42	42-43	42-44	43-46	44-45	45-46			
46-48														

exact/norm bonds :

1-2	1-5	1-23	2-3	3-4	4-5	4-6	6-7	7-8	7-9	8-11	9-10	10-11	11-24	12-13
12-16	12-23	13-14	14-15	15-16	15-17	17-18	18-19	18-20	19-22	20-21	21-22			
22-24	25-26													
25-29	25-47	26-27	27-28	28-29	28-30	30-31	31-32	31-33	32-35	33-34	34-35			
35-48	36-37													
36-40	36-47	37-38	38-39	39-40	39-41	41-42	42-43	42-44	43-46	44-45	45-46			
46-48														

Match level :

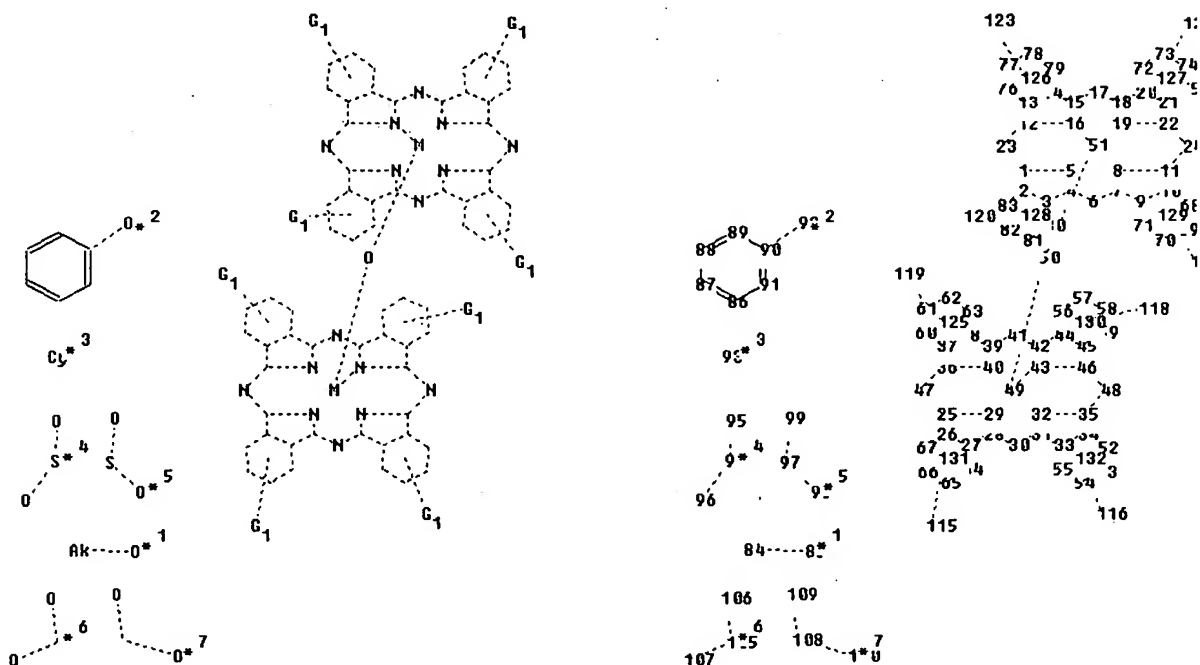
10/516884

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
 20:Atom 21:Atom
 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom
 31:Atom 32:Atom
 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom
 42:Atom 43:Atom
 44:Atom 45:Atom 46:Atom 47:Atom 48:Atom

L5 2661 SEA FILE=REGISTRY SSS FUL L4
 L15 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:
 Uploading L15b.str



chain nodes :

50 84 85 92 93 94 95 96 97 98 99 105 106 107 108 109 110 115 116
 118 119 120 121 122 123

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44
 45 46 47 48
 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72
 73 74 75
 76 77 78 79 80 81 82 83 86 87 88 89 90 91

ring/chain nodes :

10/516884

49 51

chain bonds :

49-50 50-51 84-85 90-92 94-95 94-96 97-98 97-99 105-106 105-107 108-109
108-110

ring/chain bonds :

16-51 43-49

ring bonds :

1-2 1-5 1-23 2-3 2-83 3-4 3-80 4-5 4-6 6-7 7-8 7-9 8-11 9-10 9-71
10-11 10-68 11-24 12-13 12-16 12-23 13-14 13-76 14-15 14-79 15-16 15-17
17-18 18-19 18-20
19-22 20-21 20-72 21-22 21-75 22-24 25-26 25-29 25-47 26-27 26-67 27-28
27-64 28-29
28-30 30-31 31-32 31-33 32-35 33-34 33-55 34-35 34-52 35-48 36-37 36-40
36-47 37-38
37-60 38-39 38-63 39-40 39-41 41-42 42-43 42-44 43-46 44-45 44-56 45-46
45-59 46-48
52-53 53-54 54-55 56-57 57-58 58-59 60-61 61-62 62-63 64-65 65-66 66-67
68-69 69-70
70-71 72-73 73-74 74-75 76-77 77-78 78-79 80-81 81-82 82-83 86-87 86-91
87-88 88-89
89-90 90-91

exact/norm bonds :

1-2 1-5 1-23 2-3 2-83 3-4 3-80 4-5 4-6 6-7 7-8 7-9 8-11 9-10 9-71
10-11 10-68 11-24 12-13 12-16 12-23 13-14 13-76 14-15 14-79 15-16 15-17
16-51 17-18 18-19
18-20 19-22 20-21 20-72 21-22 21-75 22-24 25-26 25-29 25-47 26-27 26-67
27-28 27-64
28-29 28-30 30-31 31-32 31-33 32-35 33-34 33-55 34-35 34-52 35-48 36-37
36-40 36-47
37-38 37-60 38-39 38-63 39-40 39-41 41-42 42-43 42-44 43-46 43-49 44-45
44-56 45-46
45-59 46-48 49-50 50-51 52-53 53-54 54-55 56-57 57-58 58-59 60-61 61-62
62-63 64-65
65-66 66-67 68-69 69-70 70-71 72-73 73-74 74-75 76-77 77-78 78-79 80-81
81-82 82-83
84-85 90-92 94-95 94-96 97-98 97-99 105-106 105-107 108-109 108-110

normalized bonds :

86-87 86-91 87-88 88-89 89-90 90-91

G1:N,CN,NO2,X,Ak, [*1], [*2], [*3], [*4], [*5], [*6], [*7]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom
22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom
31:Atom 32:Atom
33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom
42:Atom 43:Atom
44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:CLASS 50:CLASS 51:CLASS 52:Atom
53:Atom 54:Atom
55:Atom 56:Atom 57:Atom 58:Atom 59:Atom 60:Atom 61:Atom 62:Atom 63:Atom
64:Atom 65:Atom
66:Atom 67:Atom 68:Atom 69:Atom 70:Atom 71:Atom 72:Atom 73:Atom 74:Atom
75:Atom 76:Atom
77:Atom 78:Atom 79:Atom 80:Atom 81:Atom 82:Atom 83:Atom 84:CLASS 85:CLASS
86:Atom 87:Atom
88:Atom 89:Atom 90:Atom 91:Atom 92:CLASS 93:Atom 94:CLASS 95:CLASS 96:CLASS
97:CLASS

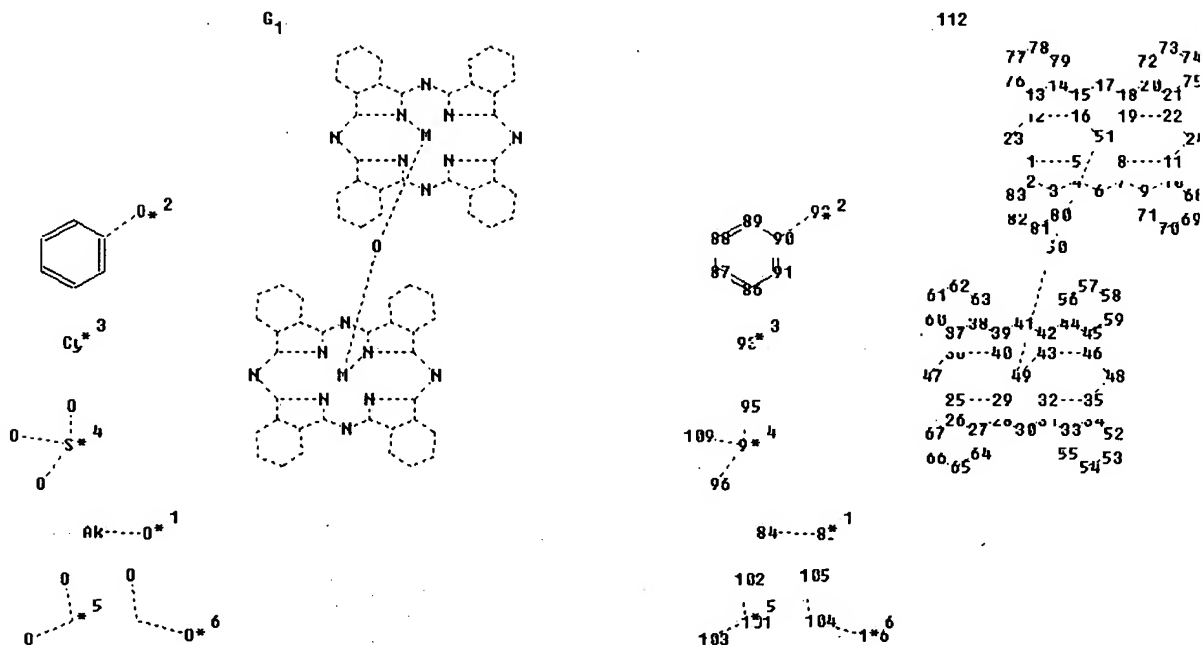
10/516884

98:CLASS 99:CLASS 105:CLASS 106:CLASS 107:CLASS 108:CLASS 109:CLASS
 110:CLASS 115:CLASS 116:CLASS
 118:CLASS 119:CLASS 120:CLASS 121:CLASS 122:CLASS 123:CLASS 125:Atom
 126:Atom 127:Atom
 128:Atom 129:Atom 130:Atom 131:Atom 132:Atom
 Generic attributes :
 93:
 Saturation : Unsaturated

L17 58 SEA FILE=REGISTRY SUB=L5 SSS FUL L15
 L32 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:
 Uploading L32b.str



chain nodes :

50 84 85 92 93 94 95 96 101 102 103 104 105 106 109 112

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44
 45 46 47 48
 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72
 73 74 75
 76 77 78 79 80 81 82 83 86 87 88 89 90 91

ring/chain nodes :

49 51

10/516884

chain bonds :

49-50 50-51 84-85 90-92 94-95 94-96 94-109 101-102 101-103 104-105 104-106

ring/chain bonds :

16-51 43-49

ring bonds :

1-2 1-5 1-23 2-3 2-83 3-4 3-80 4-5 4-6 6-7 7-8 7-9 8-11 9-10 9-71
10-11 10-68 11-24 12-13 12-16 12-23 13-14 13-76 14-15 14-79 15-16 15-17
17-18 18-19 18-20
19-22 20-21 20-72 21-22 21-75 22-24 25-26 25-29 25-47 26-27 26-67 27-28
27-64 28-29
28-30 30-31 31-32 31-33 32-35 33-34 33-55 34-35 34-52 35-48 36-37 36-40
36-47 37-38
37-60 38-39 38-63 39-40 39-41 41-42 42-43 42-44 43-46 44-45 44-56 45-46
45-59 46-48
52-53 53-54 54-55 56-57 57-58 58-59 60-61 61-62 62-63 64-65 65-66 66-67
68-69 69-70
70-71 72-73 73-74 74-75 76-77 77-78 78-79 80-81 81-82 82-83 86-87 86-91
87-88 88-89
89-90 90-91

exact/norm bonds :

1-2 1-5 1-23 2-3 2-83 3-4 3-80 4-5 4-6 6-7 7-8 7-9 8-11 9-10 9-71
10-11 10-68 11-24 12-13 12-16 12-23 13-14 13-76 14-15 14-79 15-16 15-17
16-51 17-18 18-19
18-20 19-22 20-21 20-72 21-22 21-75 22-24 25-26 25-29 25-47 26-27 26-67
27-28 27-64
28-29 28-30 30-31 31-32 31-33 32-35 33-34 33-55 34-35 34-52 35-48 36-37
36-40 36-47
37-38 37-60 38-39 38-63 39-40 39-41 41-42 42-43 42-44 43-46 43-49 44-45
44-56 45-46
45-59 46-48 49-50 50-51 52-53 53-54 54-55 56-57 57-58 58-59 60-61 61-62
62-63 64-65
65-66 66-67 68-69 69-70 70-71 72-73 73-74 74-75 76-77 77-78 78-79 80-81
81-82 82-83
84-85 90-92 94-95 94-96 94-109 101-102 101-103 104-105 104-106

normalized bonds :

86-87 86-91 87-88 88-89 89-90 90-91

G1:X,Ak,CN,NO2,N,[*1],[*2],[*3],[*4],[*5],[*6]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom
22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom
31:Atom 32:Atom
33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom
42:Atom 43:Atom
44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:CLASS 50:CLASS 51:CLASS 52:Atom
53:Atom 54:Atom
55:Atom 56:Atom 57:Atom 58:Atom 59:Atom 60:Atom 61:Atom 62:Atom 63:Atom
64:Atom 65:Atom
66:Atom 67:Atom 68:Atom 69:Atom 70:Atom 71:Atom 72:Atom 73:Atom 74:Atom
75:Atom 76:Atom
77:Atom 78:Atom 79:Atom 80:Atom 81:Atom 82:Atom 83:Atom 84:CLASS 85:CLASS
86:Atom 87:Atom
88:Atom 89:Atom 90:Atom 91:Atom 92:CLASS 93:Atom 94:CLASS 95:CLASS 96:CLASS
101:CLASS

10/516884

102:CLASS 103:CLASS 104:CLASS 105:CLASS 106:CLASS 109:CLASS 112:CLASS

Generic attributes :

93:

Saturation : Unsaturated

L34 154 SEA FILE=REGISTRY SUB=L5 SSS FUL L32
L36 8 SEA FILE=REGISTRY ABB=ON PLU=ON L17 AND NC>1
L37 1 SEA FILE=REGISTRY ABB=ON PLU=ON L36 AND HYDROXIDE/CNS
L38 1 SEA FILE=ZCAPLUS ABB=ON PLU=ON L37
L40 1 SEA FILE=REGISTRY ABB=ON PLU=ON L17 AND HYDROXIDE/CNS
L41 6 SEA FILE=REGISTRY ABB=ON PLU=ON L34 AND HYDROXIDE/CNS
L42 1 SEA FILE=REGISTRY ABB=ON PLU=ON L34 AND SULFATE/CNS
L44 154 SEA FILE=REGISTRY ABB=ON PLU=ON L17 OR L34
L46 7 SEA FILE=REGISTRY ABB=ON PLU=ON (L40 OR L41 OR L42)
L50 5 SEA FILE=ZCAPLUS ABB=ON PLU=ON L46
L57 1 SEA FILE=REGISTRY ABB=ON PLU=ON HYDROXIDE/CN
L58 1 SEA FILE=REGISTRY ABB=ON PLU=ON SULFATE/CN
L59 1 SEA FILE=REGISTRY ABB=ON PLU=ON CHLORIDE/CN
L60 0 SEA FILE=REGISTRY ABB=ON PLU=ON H S O/ELF
L61 30961 SEA FILE=REGISTRY ABB=ON PLU=ON H O S/ELF
L62 30964 SEA FILE=REGISTRY ABB=ON PLU=ON (L57 OR L58 OR L59 OR L60 OR
L61)
L63 83 SEA FILE=ZCAPLUS ABB=ON PLU=ON L44
L64 50 SEA FILE=ZCAPLUS ABB=ON PLU=ON L17
L65 4 SEA FILE=ZCAPLUS ABB=ON PLU=ON L62 AND (L63 OR L64)
L66 4 SEA FILE=ZCAPLUS ABB=ON PLU=ON L65 NOT L50
L67 1 SEA FILE=ZCAPLUS ABB=ON PLU=ON L66 AND SULFATE/OBI
L68 581403 SEA FILE=ZCAPLUS ABB=ON PLU=ON CHARGE/BI
L69 8 SEA FILE=ZCAPLUS ABB=ON PLU=ON (L63 OR L64) AND L68
L70 362 SEA FILE=ZCAPLUS ABB=ON PLU=ON TAKAKI K?/AU
L71 929 SEA FILE=ZCAPLUS ABB=ON PLU=ON YAMASAKI Y?/AU
L73 3 SEA FILE=ZCAPLUS ABB=ON PLU=ON (L70 OR L71) AND (L38 OR L50
OR L67 OR L69)

=> s L72 or L73

L74 7 L72 OR L73

=> d ibib abs hitind hitstr L74 1-7

L74 ANSWER 1 OF 7 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:1164379 ZCAPLUS Full-text

DOCUMENT NUMBER: 144:285084

TITLE: Synthesis of μ -oxo-bridged hetero-metal
phthalocyanine dimer analogues and application for
charge generating material in photoreceptor

AUTHOR(S): **Yamasaki, Yasuhiro; Takaki, Kenji**

CORPORATE SOURCE: Research Division, Orient Chemical Industries Limited,
8-1 Sanra-Higashi-Machi, Neyagawa, Osaka, 572-8581,
Japan

SOURCE: Dyes and Pigments (2005), Volume Date 2006, 70(2),
105-109

CODEN: DYPIDX; ISSN: 0143-7208

PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

10/516884

OTHER SOURCE(S): CASREACT 144:285084

AB The concentrated H₂SO₄ treatment of an equimolar mixture of a halo-(aluminum or gallium) phthalocyanine and an oxo (titanium or vanadium) phthalocyanine followed by treating in a basic solution gives selectively μ -oxo-bridged hetero-metal phthalocyanine dimer (MM'Pc)₂O in good yield. This methodol. can also serve μ -oxo-bridged hetero-metal phthalocyanine and naphthalocyanine mixed dimers. The gallium titanium hetero-metal phthalocyanine showed good photoreceptor properties.

CC 78-7 (Inorganic Chemicals and Reactions)

Section cross-reference(s): 74

IT 634179-08-1P 634179-09-2P 634179-10-5P 634179-11-6P 685834-15-5P
685834-17-7P 685834-21-3P 685834-24-6P 685834-28-0P
878274-94-3P 878274-95-4P 878275-02-6P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of μ -oxo-bridged hetero-metal phthalocyanine and naphthalocyanine dimers)

IT **878274-94-3P 878274-95-4P 878275-02-6P**

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of μ -oxo-bridged hetero-metal phthalocyanine and naphthalocyanine dimers)

RN 878274-94-3 ZCAPLUS

CN Titanium(1+), μ -oxo[[29H,31H-phthalocyaninato(2-)-
κN29,κN30,κN31,κN32]gallium][2,9,16,23-
tetrakis(1,1-dimethylethyl)-29H,31H-phthalocyaninato(2-)-
κN29,κN30,κN31,κN32]-, hydroxide (9CI) (CA INDEX
NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 878274-95-4 ZCAPLUS

CN Titanium(1+), μ -oxo[2,9,16,23-tetrakis(1,1-dimethylethyl)-29H,31H-
phthalocyaninato(2-)-κN29,κN30,κN31,κN32][[2,9,16,
23-tetrakis(1,1-dimethylethyl)-29H,31H-phthalocyaninato(2-)-
κN29,κN30,κN31,κN32]gallium]-, hydroxide (9CI)
(CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 878275-02-6 ZCAPLUS

CN Titanium(1+), μ -oxo[[2,9,16,23-tetrakis(1,1-dimethylethyl)-29H,31H-
phthalocyaninato(2-)-κN29,κN30,κN31,κN32]gallium][
37H,39H-tetranaphtho[2,3-b:2',3'-g:2'',3''-l:2''',3'''-q]porphyrizinato(2-
)-κN37,κN38,κN39,κN40]-, hydroxide (9CI) (CA
INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L74 ANSWER 2 OF 7 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:545745 ZCAPLUS Full-text

DOCUMENT NUMBER: 141:96615

TITLE: Organic electrophotographic photoreceptor

INVENTOR(S): Yamasaki, Yasuhiro; Takaki, Kenji

PATENT ASSIGNEE(S): Orient Chemical Industries, Ltd., Japan

SOURCE: Eur. Pat. Appl., 30 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

10/516884

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1435545	A1	20040707	EP 2004-50	20040105
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2004212725	A	20040729	JP 2003-523	20030106
US 2004146793	A1	20040729	US 2004-750828	20040105
US 7163772	B2	20070116		
KR 2004063813	A	20040714	KR 2004-546	20040106
PRIORITY APPLN. INFO.:			JP 2003-523	A 20030106
OTHER SOURCE(S): MARPAT 141:96615				

AB The present invention provides an organic electrophotog. photoreceptor having a conductive substrate and a photosensitive layer laid on the conductive substrate, wherein the photosensitive layer contains at least one μ -oxo bridged heterometal compound as a charge generating material. The organic electrophotog. photoreceptor has high photo-sensitivity, high stability, excellent durability on sensitivity and on elec. potential, and has excellent organic photoconductive property.

IC ICM G03G005-06
ICS C09B067-22; C09B067-00; C09B047-08; C07D487-22; C07D259-00; C07D209-00

CC 74-3 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L74 ANSWER 3 OF 7 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:386613 ZCAPLUS Full-text

DOCUMENT NUMBER: 140:398881

TITLE: Selective preparation of μ -oxo bridged heterobimetallic dinuclear naphthalocyanine and phthalocyanine compounds

INVENTOR(S): *Yamasaki, Yasuhiro; Takaki, Kenji*

PATENT ASSIGNEE(S): Orient Chemical Industries, Ltd., Japan

SOURCE: Eur. Pat. Appl., 35 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1418207	A1	20040512	EP 2003-25734	20031110
EP 1418207	B1	20070530		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2004155996	A	20040603	JP 2002-325347	20021108
US 2004091742	A1	20040513	US 2003-701610	20031106
US 7087747	B2	20060808		
PRIORITY APPLN. INFO.:			JP 2002-325347	A 20021108
OTHER SOURCE(S): MARPAT 140:398881				

AB An object of the present invention is to provide a new μ -oxo bridged heterometal compound, which can make photo-functional materials having diversified properties, and a production method such that the μ -oxo bridged heterometal compound is obtained simply, selectively and with high yield. The present invention provides μ -oxo bridged heterometal compds., NcM1-O-M2Nc ,

PcM1-O-M2Nc and NcM1-O-M2Pc wherein H2Nc represents naphthalocyanine, H2Pc represents phthalocyanine, M1 represents a metal atom (such as Al or Ga) which is able to have a valence of up to three, and M2 represents a metal atom (such as Ti or V) which is able to have a valence of four or five. Thus, [NcGa- μ -O-TiPc](OH) was prepared in 64% yield from chlorogallium naphthalocyanine [ClGaNc] and titanyl phthalocyanine [O:TiPc].

IC ICM C09B067-22
ICS C09B067-00; G03G005-06; C09B047-08; C07D487-22; C07D259-00;
C07D209-00

CC 78-7 (Inorganic Chemicals and Reactions)

IT 7429-90-5DP, Aluminum, heterobimetallic naphthalocyanine/phthalocyanine complexes 7440-32-6DP, Titanium, heterobimetallic naphthalocyanine/phthalocyanine complexes 7440-55-3DP, Gallium, heterobimetallic naphthalocyanine/phthalocyanine complexes 7440-62-2DP, Vanadium, heterobimetallic naphthalocyanine/phthalocyanine complexes 685834-15-5P 685834-17-7P 685834-21-3P 685834-23-5P 685834-24-6P 685834-26-8P 685834-28-0P **686290-60-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(selective preparation of μ -oxo bridged heterobimetallic dinuclear naphthalocyanine and phthalocyanine complexes)

IT **686290-60-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(selective preparation of μ -oxo bridged heterobimetallic dinuclear naphthalocyanine and phthalocyanine complexes)

RN 686290-60-8 ZCAPLUS

CN Titanium(1+), μ -oxo[[C,C,C,C-tetrakis(1,1-dimethylethyl)-29H,31H-phthalocyaninato(2-)- κ N29, κ N30, κ N31, κ N32]gallium][37H,39H-tetranaphtho[2,3-b:2',3'-g:2'',3''-l:2''',3'''-q]porphyrazinato(2-)- κ N37, κ N38, κ N39, κ N40]-, hydroxide (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L74 ANSWER 4 OF 7 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:991587 ZCAPLUS Full-text

DOCUMENT NUMBER: 140:28629

TITLE: μ -Oxo crosslinked dissimilar metal phthalocyanine compound and process for selectively producing the same

INVENTOR(S): **Takaki, Kenji; Yamasaki, Yasuhiro**

PATENT ASSIGNEE(S): Orient Chemical Industries, Ltd., Japan

SOURCE: PCT Int. Appl., 41 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----
WO 2003104334	A1	20031218	WO 2003-JP7240	20030609
W: JP, KR, US				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR				
EP 1514904	A1	20050316	EP 2003-730862	20030609
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, SK				

10/516884

US 2006020129	A1	20060126	US 2004-516884	20041203
PRIORITY APPLN. INFO.:			JP 2002-168580	A 20020610
			WO 2003-JP7240	W 20030609

OTHER SOURCE(S): MARPAT 140:28629

AB The present invention relates to a novel μ -oxo crosslinked dissimilar metal phthalocyanine compound useful as a **charge** generating material and a process for selectively producing the μ -oxo crosslinked dissimilar metal phthalocyanine compound in a simple manner with high yield. This μ -oxo crosslinked dissimilar metal phthalocyanine compound comprises a metal phthalocyanine containing central metal M1 and a metal phthalocyanine containing central metal M2, the central metals M1 and M2 oxo crosslinked to each other. Thus, 0.010 mol chlorogallium phthalocyanine obtained from phthalonitrile and gallium trichloride and 0.010 mol titanyl phthalocyanine obtained from phthalonitrile and titanium tetrachloride were reacted in concentrate H₂SO₄ and washed with water and further with aqueous ammonia to give μ -oxo crosslinked dissimilar metal phthalocyanine with yield 91.0%.

IC ICM C09B047-12

ICS C09B047-067; C09B047-08; C07D487-22; G03G005-06

CC 41-7 (Dyes, Organic Pigments, Fluorescent Brighteners, and Photographic Sensitizers)

Section cross-reference(s): 74

ST oxo crosslinked dissimilar metal phthalocyanine selective prepn; chlorogallium phthalocyanine titanyl phthalocyanine dimer **charge** generating material prepn

IT 634179-07-0P 634179-08-1P 634179-09-2P 634179-10-5P 634179-11-6P
634179-47-8P 634179-48-9P

RL: IMF (Industrial manufacture); PREP (Preparation)

(preparation of μ -oxo crosslinked dissimilar metal phthalocyanine compds.)

IT 634179-47-8P 634179-48-9P

RL: IMF (Industrial manufacture); PREP (Preparation)

(preparation of μ -oxo crosslinked dissimilar metal phthalocyanine compds.)

RN 634179-47-8 ZCAPLUS

CN Titanium(1+), μ -oxo[[29H,31H-phthalocyaninato(2-)-
κN29,κN30,κN31,κN32]gallium][C,C,C,C-tetrakis(1,1-
dimethylethyl)-29H,31H-phthalocyaninato(2-)-κN29,κN30,κN
31,κN32]-, hydroxide (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 634179-48-9 ZCAPLUS

CN Titanium(1+), μ -oxo[C,C,C,C-tetrakis(1,1-dimethylethyl)-29H,31H-
phthalocyaninato(2-)-κN29,κN30,κN31,κN32][[C,C,C,C-
tetrakis(1,1-dimethylethyl)-29H,31H-phthalocyaninato(2-)-
κN29,κN30,κN31,κN32]gallium]-, hydroxide (9CI)
(CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L74 ANSWER 5 OF 7 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:367072 ZCAPLUS Full-text

DOCUMENT NUMBER: 133:18773

TITLE: Oxoaluminum/gallium phthalocyanine dimers

INVENTOR(S): Yamasaki, Yasuhiro; Takaki, Kenji;

Kuroda, Kazuyoshi

PATENT ASSIGNEE(S): Orient Chemical Industries, Ltd., Japan

10/516884

SOURCE: Eur. Pat. Appl., 23 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1004634	A2	20000531	EP 1999-123213	19991125
EP 1004634	A3	20020306		
EP 1004634	B1	20031008		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
US 6093514	A	20000725	US 1999-444697	19991124
JP 2000219817	A	20000808	JP 1999-334128	19991125
PRIORITY APPLN. INFO.:			JP 1998-335729	A 19981126

AB The μ -oxoaluminum/gallium phthalocyanine dimers and their mixed crystals are suitable as a charge generating material for an organic photoconductive material, such as an electrophotog. photoreceptor. Thus, hydrolyzing a mixture of 0.01 mol chlorogallium phthalocyanine and 0.01 mol. chloroaluminum phthalocyanine with concentrate H₂SO₄ followed by dehydrating the resulting hydroxymetal phthalocyanine mixture gave an μ -oxo- aluminum/gallium phthalocyanine dimer.

IC ICM C09B067-22

ICS C09B047-04; G03G005-06

CC 41-7 (Dyes, Organic Pigments, Fluorescent Brighteners, and Photographic Sensitizers)

Section cross-reference(s): 74

L74 ANSWER 6 OF 7 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1999:815646 ZCAPLUS Full-text

DOCUMENT NUMBER: 132:144318

TITLE: μ -Oxo-bridged type aluminum and gallium phthalocyanine dimer - Synthesis, polymorphs and its primary evaluation as an electrophotographic receptor

AUTHOR(S): Yamasaki, Yasuhiro; Takaki, Kenji;

Kuroda, Kazuyoshi

CORPORATE SOURCE: 3rd R & D Center, R & D Department, Orient Chemical Industries, Ltd., Neyagawa-shi, 572-8581, Japan

SOURCE: Nippon Kagaku Kaishi (1999), (12), 841-845

CODEN: NKAKB8; ISSN: 0369-4577

PUBLISHER: Nippon Kagakkai

DOCUMENT TYPE: Journal

LANGUAGE: Japanese

AB We already found and reported that the specific polymorphs of μ -oxo-aluminum phthalocyanine dimer and μ -oxo-gallium phthalocyanine dimer have fairly good characteristics as the electrophotog. receptor. In connection with our ongoing works on this field, we are interested in the synthesis of μ -oxo-bridged dimers of diverse metal phthalocyanines for pursuing various charge generating materials in electrophotog. receptors. We report here the results of studies on the polymorphs of the titled phthalocyanine dimer, ie. μ -oxo-bridged between aluminum and gallium phthalocyanine dimer, and their primary electrophotog. evaluation.

CC 74-3 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)

Section cross-reference(s): 29, 75, 78

L74 ANSWER 7 OF 7 ZCAPLUS COPYRIGHT 2007 ACS on STN

10/516884

ACCESSION NUMBER: 1997:804467 ZCAPLUS Full-text

DOCUMENT NUMBER: 128:83612

TITLE: Synthesis of new polymorphs of μ -oxo-metal(III) phthalocyanine dimers and their photoconductive properties

AUTHOR(S): *Yamasaki, Yasuhiro*; Kuroda, Kazuyoshi; *Takaki, Kenji*

CORPORATE SOURCE: I-2 Group, R & D Dep., Orient Chem. Industries, Ltd., Osaka, 572, Japan

SOURCE: Nippon Kagaku Kaishi (1997), (12), 887-898
CODEN: NKAKB8; ISSN: 0369-4577

PUBLISHER: Nippon Kagakkai

DOCUMENT TYPE: Journal

LANGUAGE: Japanese

AB [MPc]20 (M = Al, Ga; H2Pc = phthalocyanine) were prepared and studied their polymorphs through x-ray diffraction anal. [MPc]20 have several polymorphs, but one of the target compds., that is [InPc]20, could not be synthesized because InPcCl was easily hydrolyzed through acid-pasting treatment procedure to give metal-free phthalocyanine. The characterization of these compds. by the several chemical anal. methods was satisfied for the target mols. and the FD-Mass anal. distinguished clearly between the hydroxymetal phthalocyanine and the corresponding phthalocyanine dimer. The authors also studied their photoconductive properties on the bilayer photoreceptor consisted of the above phthalocyanine dimer as the charge generating material. The specific polymorphs of [AlPc]20-II have good spectral response of the photosensitivity in the shorter wavelength, and the [GaPc]20-G has a fairly high photosensitivity in the wavelength region of laser diode light wavelength, compared with the common phthalocyanine photoreceptors.

CC 78-7 (Inorganic Chemicals and Reactions)

Section cross-reference(s): 72, 73, 74

10/516884

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FILE COVERS 1907 - 7 Dec 2007 VOL 147 ISS 25
FILE LAST UPDATED: 6 Dec 2007 (20071206/ED)

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This file contains CAS Registry Numbers for easy and accurate
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'OBI' IS DEFAULT SEARCH FIELD FOR 'ZCAPLUS' FILE

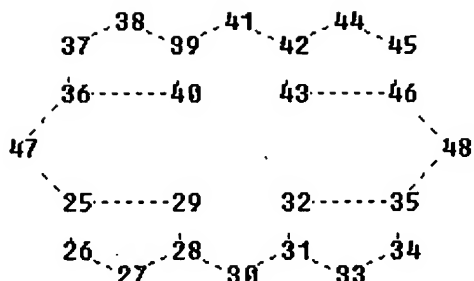
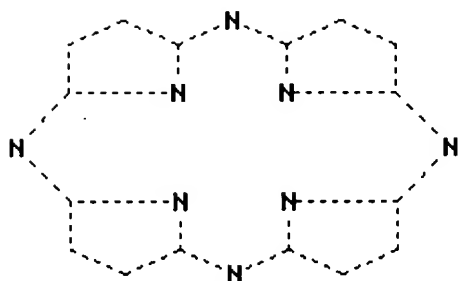
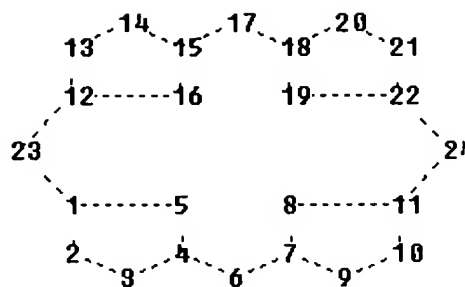
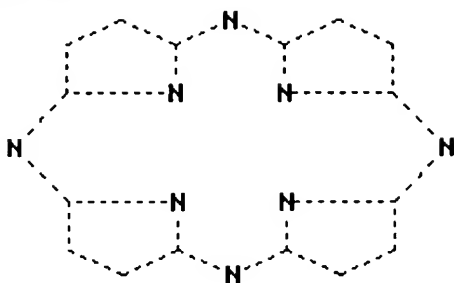
=> d stat que L38
L4 STR

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Structure attributes must be viewed using STN Express query preparation:

10/516884

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ring nodes :

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23		
24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48

ring bonds :

1-2	1-5	1-23	2-3	3-4	4-5	4-6	6-7	7-8	7-9	8-11	9-10	10-11	11-24	12-13
12-16	12-23	13-14	14-15	15-16	15-17	17-18	18-19	18-20	19-22	20-21	21-22	22-24	25-26	
25-29	25-47	26-27	27-28	28-29	28-30	30-31	31-32	31-33	32-35	33-34	34-35	35-48	36-37	
36-40	36-47	37-38	38-39	39-40	39-41	41-42	42-43	42-44	43-46	44-45	45-46	46-48		

exact/norm bonds :

1-2	1-5	1-23	2-3	3-4	4-5	4-6	6-7	7-8	7-9	8-11	9-10	10-11	11-24	12-13
12-16	12-23	13-14	14-15	15-16	15-17	17-18	18-19	18-20	19-22	20-21	21-22	22-24	25-26	
25-29	25-47	26-27	27-28	28-29	28-30	30-31	31-32	31-33	32-35	33-34	34-35	35-48	36-37	
36-40	36-47	37-38	38-39	39-40	39-41	41-42	42-43	42-44	43-46	44-45	45-46	46-48		

Match level :

1:Atom	2:Atom	3:Atom	4:Atom	5:Atom	6:Atom	7:Atom	8:Atom	9:Atom	10:Atom	11:Atom	12:Atom	13:Atom	14:Atom	15:Atom	16:Atom	17:Atom	18:Atom	19:Atom	20:Atom	21:Atom	22:Atom	23:Atom	24:Atom	25:Atom	26:Atom	27:Atom	28:Atom	29:Atom	30:Atom	31:Atom	32:Atom
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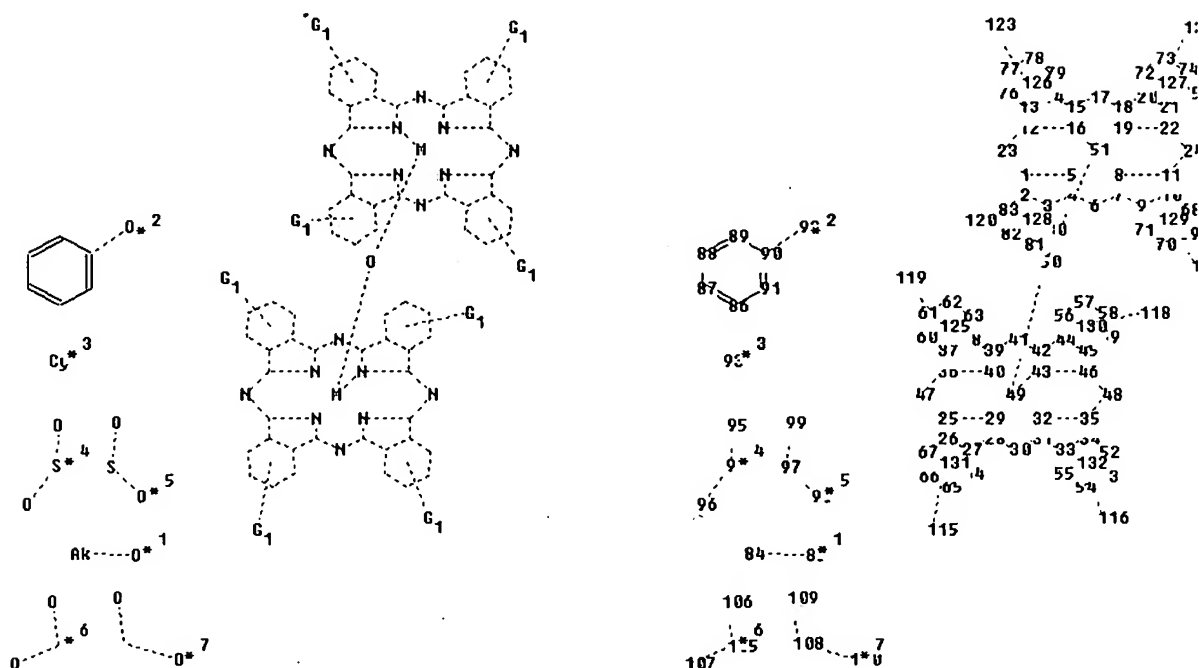
10/516884

33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom
42:Atom 43:Atom
44:Atom 45:Atom 46:Atom 47:Atom 48:Atom

L5 2661 SEA FILE=REGISTRY SSS FUL L4
L15 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:
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chain nodes :

50 84 85 92 93 94 95 96 97 98 99 105 106 107 108 109 110 115 116
118 119 120 121 122 123

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44
45 46 47 48
52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72
73 74 75
76 77 78 79 80 81 82 83 86 87 88 89 90 91

ring/chain nodes :

49 51

chain bonds :

49-50 50-51 84-85 90-92 94-95 94-96 97-98 97-99 105-106 105-107 108-109
108-110

ring/chain bonds :

10/516884

16-51 43-49

ring bonds :

1-2 1-5 1-23 2-3 2-83 3-4 3-80 4-5 4-6 6-7 7-8 7-9 8-11 9-10 9-71
10-11 10-68 11-24 12-13 12-16 12-23 13-14 13-76 14-15 14-79 15-16 15-17
17-18 18-19 18-20
19-22 20-21 20-72 21-22 21-75 22-24 25-26 25-29 25-47 26-27 26-67 27-28
27-64 28-29
28-30 30-31 31-32 31-33 32-35 33-34 33-55 34-35 34-52 35-48 36-37 36-40
36-47 37-38
37-60 38-39 38-63 39-40 39-41 41-42 42-43 42-44 43-46 44-45 44-56 45-46
45-59 46-48
52-53 53-54 54-55 56-57 57-58 58-59 60-61 61-62 62-63 64-65 65-66 66-67
68-69 69-70
70-71 72-73 73-74 74-75 76-77 77-78 78-79 80-81 81-82 82-83 86-87 86-91
87-88 88-89
89-90 90-91

exact/norm bonds :

1-2 1-5 1-23 2-3 2-83 3-4 3-80 4-5 4-6 6-7 7-8 7-9 8-11 9-10 9-71
10-11 10-68 11-24 12-13 12-16 12-23 13-14 13-76 14-15 14-79 15-16 15-17
16-51 17-18 18-19
18-20 19-22 20-21 20-72 21-22 21-75 22-24 25-26 25-29 25-47 26-27 26-67
27-28 27-64
28-29 28-30 30-31 31-32 31-33 32-35 33-34 33-55 34-35 34-52 35-48 36-37
36-40 36-47
37-38 37-60 38-39 38-63 39-40 39-41 41-42 42-43 42-44 43-46 43-49 44-45
44-56 45-46
45-59 46-48 49-50 50-51 52-53 53-54 54-55 56-57 57-58 58-59 60-61 61-62
62-63 64-65
65-66 66-67 68-69 69-70 70-71 72-73 73-74 74-75 76-77 77-78 78-79 80-81
81-82 82-83
84-85 90-92 94-95 94-96 97-98 97-99 105-106 105-107 108-109 108-110
normalized bonds :
86-87 86-91 87-88 88-89 89-90 90-91

G1:N,CN,NO2,X,Ak, [*1], [*2], [*3], [*4], [*5], [*6], [*7]

Match level :

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11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom
22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom
31:Atom 32:Atom
33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom
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44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:CLASS 50:CLASS 51:CLASS 52:Atom
53:Atom 54:Atom
55:Atom 56:Atom 57:Atom 58:Atom 59:Atom 60:Atom 61:Atom 62:Atom 63:Atom
64:Atom 65:Atom
66:Atom 67:Atom 68:Atom 69:Atom 70:Atom 71:Atom 72:Atom 73:Atom 74:Atom
75:Atom 76:Atom
77:Atom 78:Atom 79:Atom 80:Atom 81:Atom 82:Atom 83:Atom 84:CLASS 85:CLASS
86:Atom 87:Atom
88:Atom 89:Atom 90:Atom 91:Atom 92:CLASS 93:Atom 94:CLASS 95:CLASS 96:CLASS
97:CLASS
98:CLASS 99:CLASS 105:CLASS 106:CLASS 107:CLASS 108:CLASS 109:CLASS
110:CLASS 115:CLASS 116:CLASS
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126:Atom 127:Atom
128:Atom 129:Atom 130:Atom 131:Atom 132:Atom

10/516884

Generic attributes :

93:

Saturation : Unsaturated

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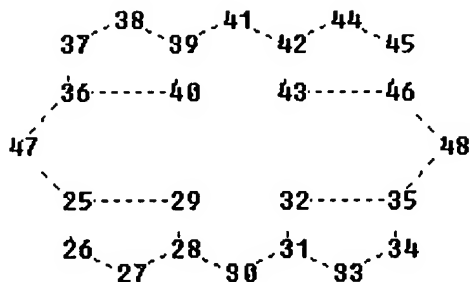
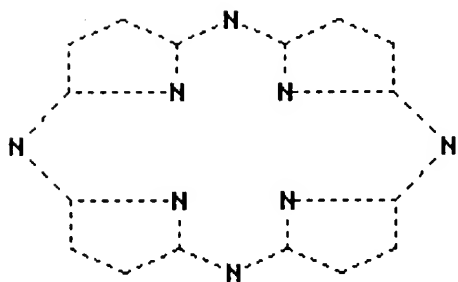
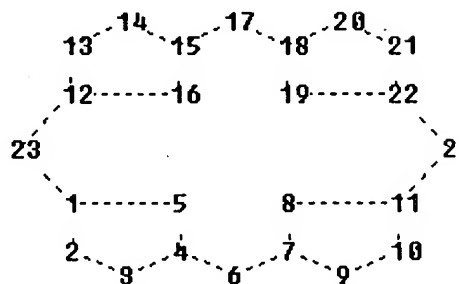
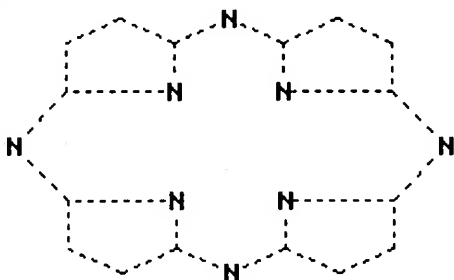
=> d stat que L50

L4 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:

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ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44
45 46 47 48

ring bonds :

1-2 1-5 1-23 2-3 3-4 4-5 4-6 6-7 7-8 7-9 8-11 9-10 10-11 11-24 12-13
12-16 12-23 13-14 14-15 15-16 15-17 17-18 18-19 18-20 19-22 20-21 21-22
22-24 25-26

10/516884

25-29 25-47 26-27 27-28 28-29 28-30 30-31 31-32 31-33 32-35 33-34 34-35
35-48 36-37
36-40 36-47 37-38 38-39 39-40 39-41 41-42 42-43 42-44 43-46 44-45 45-46
46-48
exact/norm bonds :
1-2 1-5 1-23 2-3 3-4 4-5 4-6 6-7 7-8 7-9 8-11 9-10 10-11 11-24 12-13
12-16 12-23 13-14 14-15 15-16 15-17 17-18 18-19 18-20 19-22 20-21 21-22
22-24 25-26
25-29 25-47 26-27 27-28 28-29 28-30 30-31 31-32 31-33 32-35 33-34 34-35
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46-48

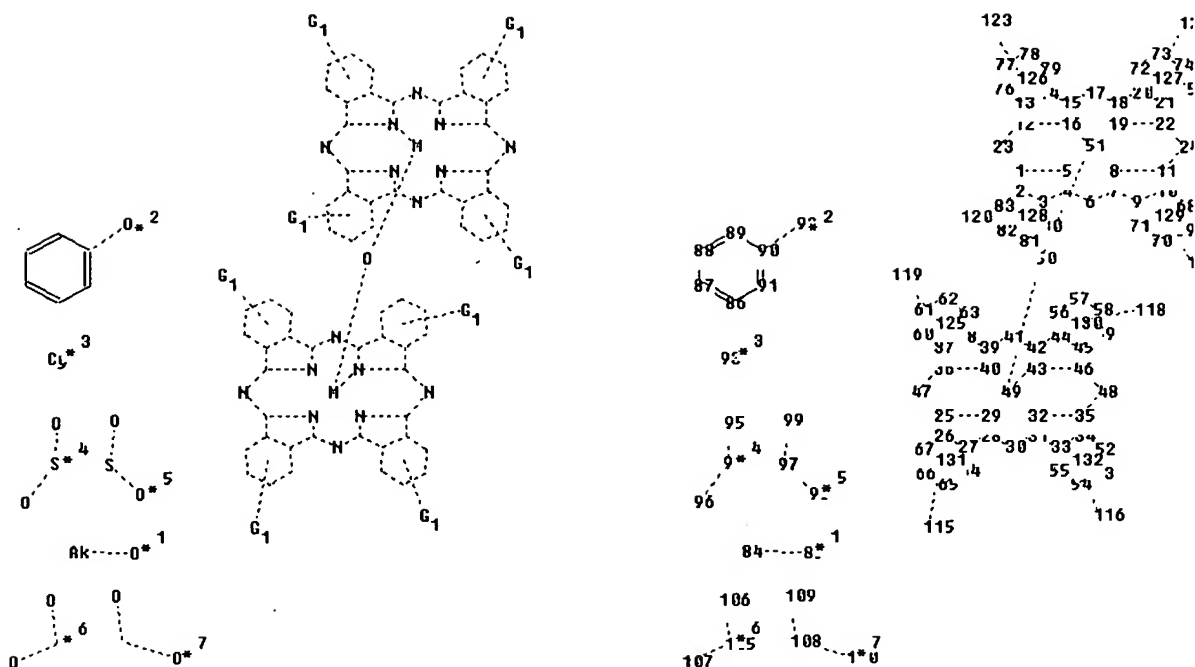
Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom
22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom
31:Atom 32:Atom
33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom
42:Atom 43:Atom
44:Atom 45:Atom 46:Atom 47:Atom 48:Atom

L5 2661 SEA FILE=REGISTRY SSS FUL L4
L15 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:
Uploading L15b.str



chain nodes :

50 84 85 92 93 94 95 96 97 98 99 105 106 107 108 109 110 115 116
118 119 120 121 122 123

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44
45 46 47 48
52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72
73 74 75
76 77 78 79 80 81 82 83 86 87 88 89 90 91

ring/chain nodes :

49 51

chain bonds :

49-50 50-51 84-85 90-92 94-95 94-96 97-98 97-99 105-106 105-107 108-109
108-110

ring/chain bonds :

16-51 43-49

ring bonds :

1-2 1-5 1-23 2-3 2-83 3-4 3-80 4-5 4-6 6-7 7-8 7-9 8-11 9-10 9-71
10-11 10-68 11-24 12-13 12-16 12-23 13-14 13-76 14-15 14-79 15-16 15-17
17-18 18-19 18-20
19-22 20-21 20-72 21-22 21-75 22-24 25-26 25-29 25-47 26-27 26-67 27-28
27-64 28-29
28-30 30-31 31-32 31-33 32-35 33-34 33-55 34-35 34-52 35-48 36-37 36-40
36-47 37-38
37-60 38-39 38-63 39-40 39-41 41-42 42-43 42-44 43-46 44-45 44-56 45-46
45-59 46-48
52-53 53-54 54-55 56-57 57-58 58-59 60-61 61-62 62-63 64-65 65-66 66-67
68-69 69-70
70-71 72-73 73-74 74-75 76-77 77-78 78-79 80-81 81-82 82-83 86-87 86-91

10/516884

87-88 88-89

89-90 90-91

exact/norm bonds :

1-2 1-5 1-23 2-3 2-83 3-4 3-80 4-5 4-6 6-7 7-8 7-9 8-11 9-10 9-71
10-11 10-68 11-24 12-13 12-16 12-23 13-14 13-76 14-15 14-79 15-16 15-17
16-51 17-18 18-19
18-20 19-22 20-21 20-72 21-22 21-75 22-24 25-26 25-29 25-47 26-27 26-67
27-28 27-64
28-29 28-30 30-31 31-32 31-33 32-35 33-34 33-55 34-35 34-52 35-48 36-37
36-40 36-47
37-38 37-60 38-39 38-63 39-40 39-41 41-42 42-43 42-44 43-46 43-49 44-45
44-56 45-46
45-59 46-48 49-50 50-51 52-53 53-54 54-55 56-57 57-58 58-59 60-61 61-62
62-63 64-65
65-66 66-67 68-69 69-70 70-71 72-73 73-74 74-75 76-77 77-78 78-79 80-81
81-82 82-83
84-85 90-92 94-95 94-96 97-98 97-99 105-106 105-107 108-109 108-110
normalized bonds :
86-87 86-91 87-88 88-89 89-90 90-91

G1:N,CN,NO2,X,Ak, [*1], [*2], [*3], [*4], [*5], [*6], [*7]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom
22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom
31:Atom 32:Atom
33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom
42:Atom 43:Atom
44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:CLASS 50:CLASS 51:CLASS 52:Atom
53:Atom 54:Atom
55:Atom 56:Atom 57:Atom 58:Atom 59:Atom 60:Atom 61:Atom 62:Atom 63:Atom
64:Atom 65:Atom
66:Atom 67:Atom 68:Atom 69:Atom 70:Atom 71:Atom 72:Atom 73:Atom 74:Atom
75:Atom 76:Atom
77:Atom 78:Atom 79:Atom 80:Atom 81:Atom 82:Atom 83:Atom 84:CLASS 85:CLASS
86:Atom 87:Atom
88:Atom 89:Atom 90:Atom 91:Atom 92:CLASS 93:Atom 94:CLASS 95:CLASS 96:CLASS
97:CLASS
98:CLASS 99:CLASS 105:CLASS 106:CLASS 107:CLASS 108:CLASS 109:CLASS
110:CLASS 115:CLASS 116:CLASS
118:CLASS 119:CLASS 120:CLASS 121:CLASS 122:CLASS 123:CLASS 125:Atom
126:Atom 127:Atom
128:Atom 129:Atom 130:Atom 131:Atom 132:Atom

Generic attributes :

93:

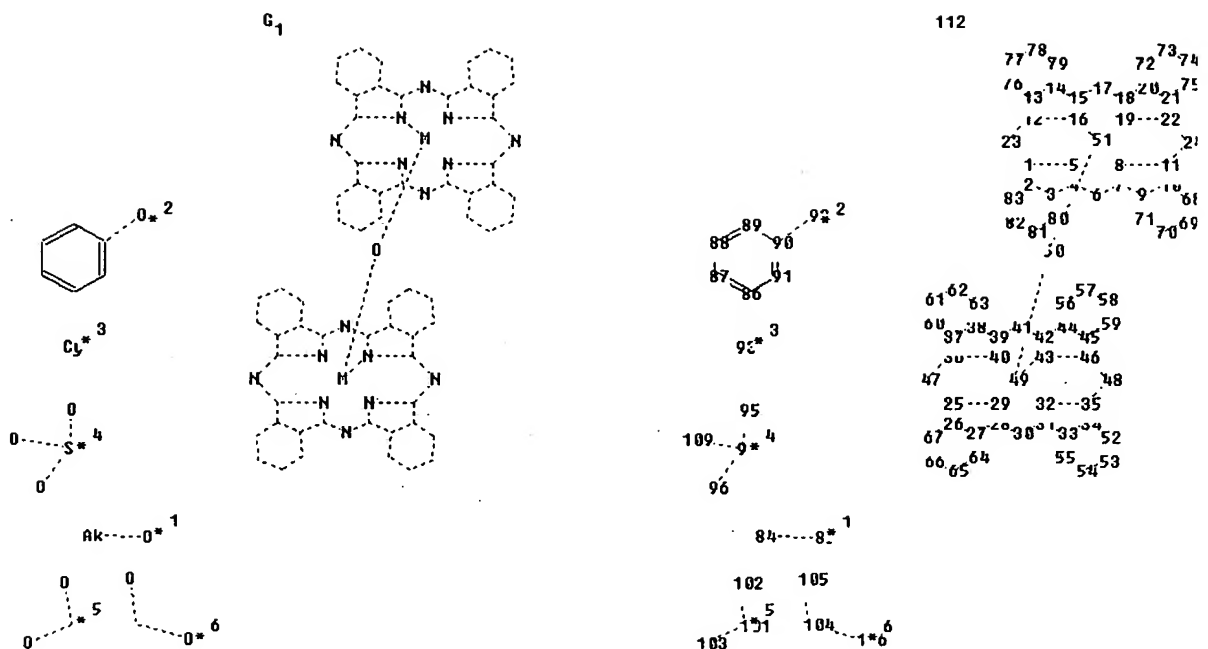
Saturation : Unsaturated

L17 58 SEA FILE=REGISTRY SUB=L5 SSS FUL L15

L32 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:



chain nodes :

50 84 85 92 93 94 95 96 101 102 103 104 105 106 109 112

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44
 45 46 47 48
 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72
 73 74 75
 76 77 78 79 80 81 82 83 86 87 88 89 90 91

ring/chain nodes :

49 51

chain bonds :

49-50 50-51 84-85 90-92 94-95 94-96 94-109 101-102 101-103 104-105 104-106

ring/chain bonds :

16-51 43-49

ring bonds :

1-2 1-5 1-23 2-3 2-83 3-4 3-80 4-5 4-6 6-7 7-8 7-9 8-11 9-10 9-71
 10-11 10-68 11-24 12-13 12-16 12-23 13-14 13-76 14-15 14-79 15-16 15-17
 17-18 18-19 18-20
 19-22 20-21 20-72 21-22 21-75 22-24 25-26 25-29 25-47 26-27 26-67 27-28
 27-64 28-29
 28-30 30-31 31-32 31-33 32-35 33-34 33-55 34-35 34-52 35-48 36-37 36-40
 36-47 37-38
 37-60 38-39 38-63 39-40 39-41 41-42 42-43 42-44 43-46 44-45 44-56 45-46
 45-59 46-48
 52-53 53-54 54-55 56-57 57-58 58-59 60-61 61-62 62-63 64-65 65-66 66-67
 68-69 69-70
 70-71 72-73 73-74 74-75 76-77 77-78 78-79 80-81 81-82 82-83 86-87 86-91

10/516884

87-88 88-89

89-90 90-91

exact/norm bonds :

1-2 1-5 1-23 2-3 2-83 3-4 3-80 4-5 4-6 6-7 7-8 7-9 8-11 9-10 9-71
10-11 10-68 11-24 12-13 12-16 12-23 13-14 13-76 14-15 14-79 15-16 15-17
16-51 17-18 18-19
18-20 19-22 20-21 20-72 21-22 21-75 22-24 25-26 25-29 25-47 26-27 26-67
27-28 27-64
28-29 28-30 30-31 31-32 31-33 32-35 33-34 33-55 34-35 34-52 35-48 36-37
36-40 36-47
37-38 37-60 38-39 38-63 39-40 39-41 41-42 42-43 42-44 43-46 43-49 44-45
44-56 45-46
45-59 46-48 49-50 50-51 52-53 53-54 54-55 56-57 57-58 58-59 60-61 61-62
62-63 64-65
65-66 66-67 68-69 69-70 70-71 72-73 73-74 74-75 76-77 77-78 78-79 80-81
81-82 82-83
84-85 90-92 94-95 94-96 94-109 101-102 101-103 104-105 104-106
normalized bonds :
86-87 86-91 87-88 88-89 89-90 90-91

G1:X,Ak,CN,NO2,N, [*1], [*2], [*3], [*4], [*5], [*6]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom
22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom
31:Atom 32:Atom
33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom
42:Atom 43:Atom
44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:CLASS 50:CLASS 51:CLASS 52:Atom
53:Atom 54:Atom
55:Atom 56:Atom 57:Atom 58:Atom 59:Atom 60:Atom 61:Atom 62:Atom 63:Atom
64:Atom 65:Atom
66:Atom 67:Atom 68:Atom 69:Atom 70:Atom 71:Atom 72:Atom 73:Atom 74:Atom
75:Atom 76:Atom
77:Atom 78:Atom 79:Atom 80:Atom 81:Atom 82:Atom 83:Atom 84:CLASS 85:CLASS
86:Atom 87:Atom
88:Atom 89:Atom 90:Atom 91:Atom 92:CLASS 93:Atom 94:CLASS 95:CLASS 96:CLASS
101:CLASS
102:CLASS 103:CLASS 104:CLASS 105:CLASS 106:CLASS 109:CLASS 112:CLASS

Generic attributes :

93:

Saturation : Unsaturated

L34 154 SEA FILE=REGISTRY SUB=L5 SSS FUL L32
L40 1 SEA FILE=REGISTRY ABB=ON PLU=ON L17 AND HYDROXIDE/CNS
L41 6 SEA FILE=REGISTRY ABB=ON PLU=ON L34 AND HYDROXIDE/CNS
L42 1 SEA FILE=REGISTRY ABB=ON PLU=ON L34 AND SULFATE/CNS
L46 7 SEA FILE=REGISTRY ABB=ON PLU=ON (L40 OR L41 OR L42)
L50 5 SEA FILE=ZCAPLUS ABB=ON PLU=ON L46

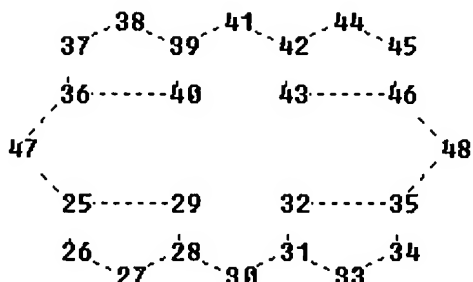
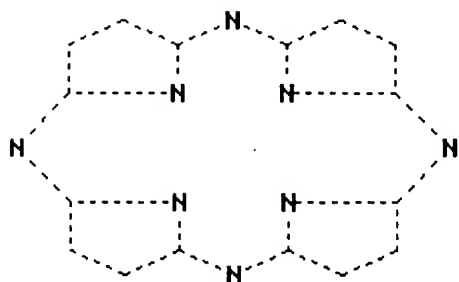
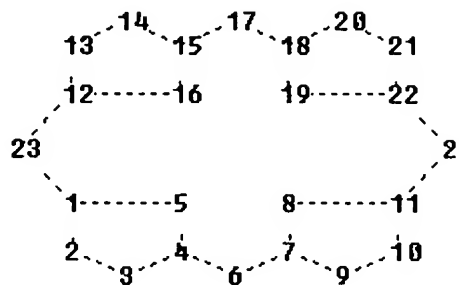
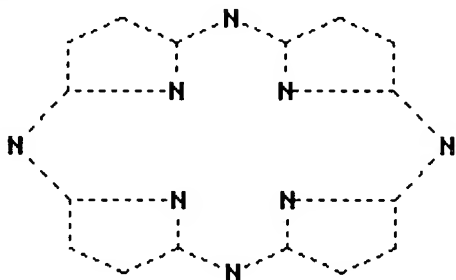
=> d stat que L67

L4 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:

Uploading L4b.str



ring nodes :

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23
24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44		
45	46	47	48																			

ring bonds :

1-2	1-5	1-23	2-3	3-4	4-5	4-6	6-7	7-8	7-9	8-11	9-10	10-11	11-24	12-13
12-16	12-23	13-14	14-15	15-16	15-17	17-18	18-19	18-20	19-22	20-21	21-22			
22-24	25-26													
25-29	25-47	26-27	27-28	28-29	28-30	30-31	31-32	31-33	32-35	33-34	34-35			
35-48	36-37													
36-40	36-47	37-38	38-39	39-40	39-41	41-42	42-43	42-44	43-46	44-45	45-46			
46-48														

exact/norm bonds :

1-2	1-5	1-23	2-3	3-4	4-5	4-6	6-7	7-8	7-9	8-11	9-10	10-11	11-24	12-13
12-16	12-23	13-14	14-15	15-16	15-17	17-18	18-19	18-20	19-22	20-21	21-22			
22-24	25-26													
25-29	25-47	26-27	27-28	28-29	28-30	30-31	31-32	31-33	32-35	33-34	34-35			
35-48	36-37													
36-40	36-47	37-38	38-39	39-40	39-41	41-42	42-43	42-44	43-46	44-45	45-46			
46-48														

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom

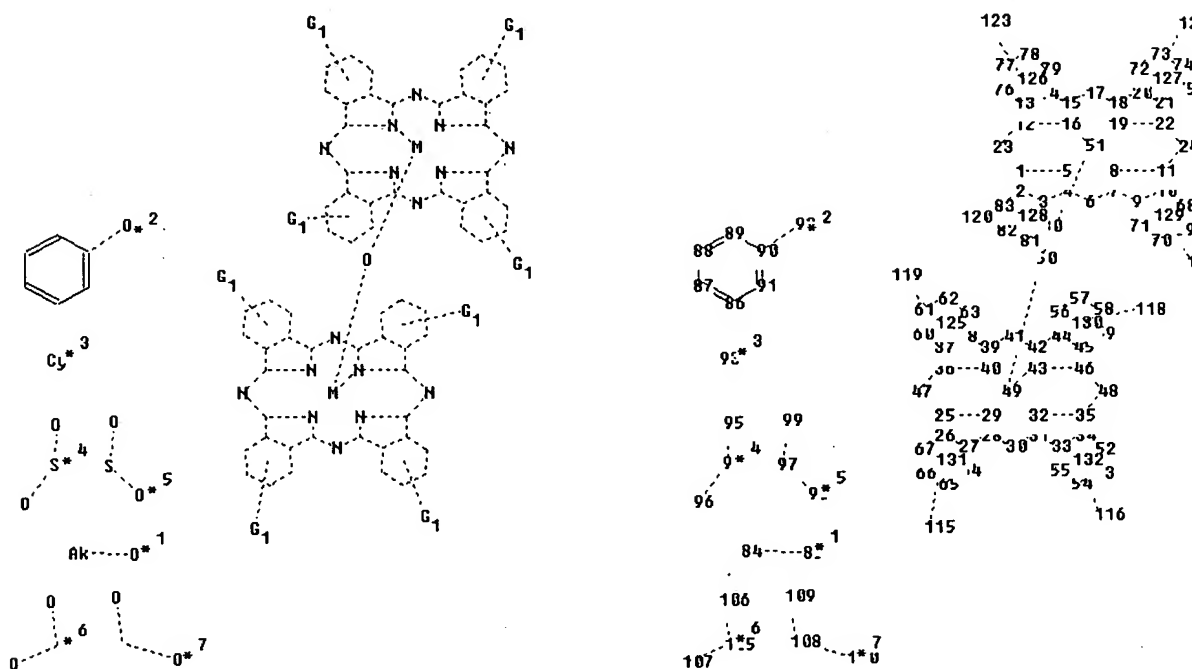
10/516884

11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
 20:Atom 21:Atom
 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom
 31:Atom 32:Atom
 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom
 42:Atom 43:Atom
 44:Atom 45:Atom 46:Atom 47:Atom 48:Atom

L5 2661 SEA FILE=REGISTRY SSS FUL L4
 L15 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:
 Uploading L15b.str



chain nodes :

50 84 85 92 93 94 95 96 97 98 99 105 106 107 108 109 110 115 116
 118 119 120 121 122 123

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44
 45 46 47 48
 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72
 73 74 75
 76 77 78 79 80 81 82 83 86 87 88 89 90 91

ring/chain nodes :

49 51

10/516884

chain bonds :

49-50 50-51 84-85 90-92 94-95 94-96 97-98 97-99 105-106 105-107 108-109
108-110

ring/chain bonds :

16-51 43-49

ring bonds :

1-2 1-5 1-23 2-3 2-83 3-4 3-80 4-5 4-6 6-7 7-8 7-9 8-11 9-10 9-71
10-11 10-68 11-24 12-13 12-16 12-23 13-14 13-76 14-15 14-79 15-16 15-17
17-18 18-19 18-20
19-22 20-21 20-72 21-22 21-75 22-24 25-26 25-29 25-47 26-27 26-67 27-28
27-64 28-29
28-30 30-31 31-32 31-33 32-35 33-34 33-55 34-35 34-52 35-48 36-37 36-40
36-47 37-38
37-60 38-39 38-63 39-40 39-41 41-42 42-43 42-44 43-46 44-45 44-56 45-46
45-59 46-48
52-53 53-54 54-55 56-57 57-58 58-59 60-61 61-62 62-63 64-65 65-66 66-67
68-69 69-70
70-71 72-73 73-74 74-75 76-77 77-78 78-79 80-81 81-82 82-83 86-87 86-91
87-88 88-89
89-90 90-91

exact/norm bonds :

1-2 1-5 1-23 2-3 2-83 3-4 3-80 4-5 4-6 6-7 7-8 7-9 8-11 9-10 9-71
10-11 10-68 11-24 12-13 12-16 12-23 13-14 13-76 14-15 14-79 15-16 15-17
16-51 17-18 18-19
18-20 19-22 20-21 20-72 21-22 21-75 22-24 25-26 25-29 25-47 26-27 26-67
27-28 27-64
28-29 28-30 30-31 31-32 31-33 32-35 33-34 33-55 34-35 34-52 35-48 36-37
36-40 36-47
37-38 37-60 38-39 38-63 39-40 39-41 41-42 42-43 42-44 43-46 43-49 44-45
44-56 45-46
45-59 46-48 49-50 50-51 52-53 53-54 54-55 56-57 57-58 58-59 60-61 61-62
62-63 64-65
65-66 66-67 68-69 69-70 70-71 72-73 73-74 74-75 76-77 77-78 78-79 80-81
81-82 82-83
84-85 90-92 94-95 94-96 97-98 97-99 105-106 105-107 108-109 108-110

normalized bonds :

86-87 86-91 87-88 88-89 89-90 90-91

G1:N,CN,NO2,X,Ak, [*1], [*2], [*3], [*4], [*5], [*6], [*7]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom
22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom
31:Atom 32:Atom
33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom
42:Atom 43:Atom
44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:CLASS 50:CLASS 51:CLASS 52:Atom
53:Atom 54:Atom
55:Atom 56:Atom 57:Atom 58:Atom 59:Atom 60:Atom 61:Atom 62:Atom 63:Atom
64:Atom 65:Atom
66:Atom 67:Atom 68:Atom 69:Atom 70:Atom 71:Atom 72:Atom 73:Atom 74:Atom
75:Atom 76:Atom
77:Atom 78:Atom 79:Atom 80:Atom 81:Atom 82:Atom 83:Atom 84:CLASS 85:CLASS
86:Atom 87:Atom
88:Atom 89:Atom 90:Atom 91:Atom 92:CLASS 93:Atom 94:CLASS 95:CLASS 96:CLASS
97:CLASS
98:CLASS 99:CLASS 105:CLASS 106:CLASS 107:CLASS 108:CLASS 109:CLASS

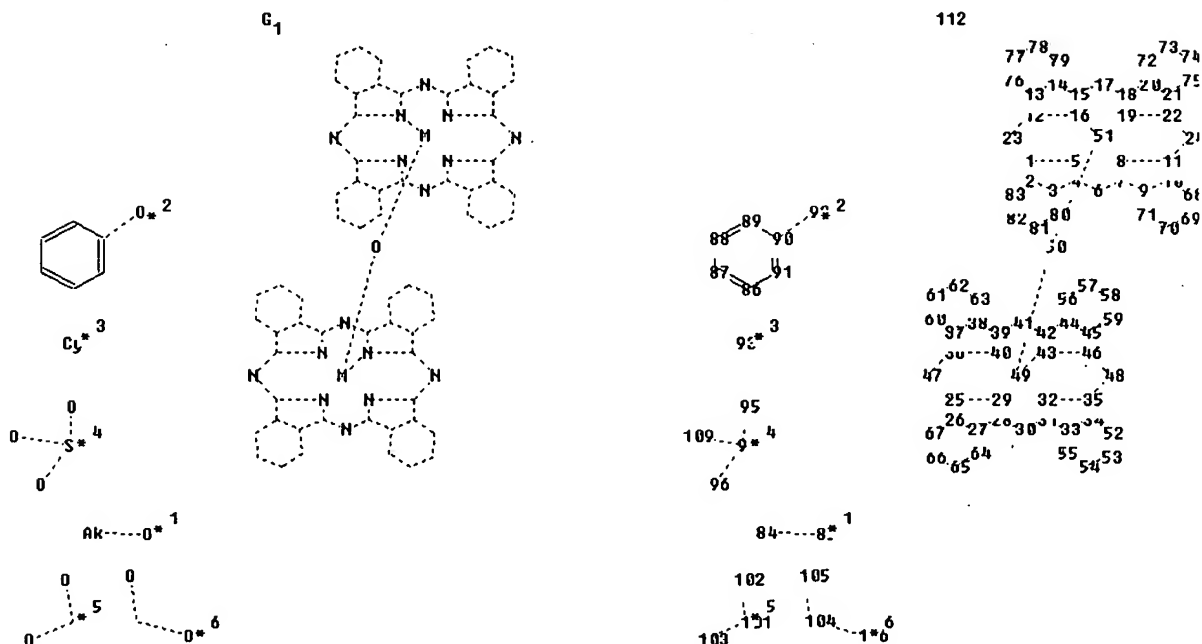
10/516884

110:CLASS 115:CLASS 116:CLASS
 118:CLASS 119:CLASS 120:CLASS 121:CLASS 122:CLASS 123:CLASS 125:Atom
 126:Atom 127:Atom
 128:Atom 129:Atom 130:Atom 131:Atom 132:Atom
 Generic attributes :
 93:
 Saturation : Unsaturated

L17 58 SEA FILE=REGISTRY SUB=L5 SSS FUL L15
 L32 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:
 Uploading L32b.str



chain nodes :

50 84 85 92 93 94 95 96 101 102 103 104 105 106 109 112

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44
 45 46 47 48
 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72
 73 74 75
 76 77 78 79 80 81 82 83 86 87 88 89 90 91

ring/chain nodes :

49 51

chain bonds :

10/516884

49-50 50-51 84-85 90-92 94-95 94-96 94-109 101-102 101-103 104-105 104-106

ring/chain bonds :

16-51 43-49

ring bonds :

1-2 1-5 1-23 2-3 2-83 3-4 3-80 4-5 4-6 6-7 7-8 7-9 8-11 9-10 9-71
10-11 10-68 11-24 12-13 12-16 12-23 13-14 13-76 14-15 14-79 15-16 15-17
17-18 18-19 18-20
19-22 20-21 20-72 21-22 21-75 22-24 25-26 25-29 25-47 26-27 26-67 27-28
27-64 28-29
28-30 30-31 31-32 31-33 32-35 33-34 33-55 34-35 34-52 35-48 36-37 36-40
36-47 37-38
37-60 38-39 38-63 39-40 39-41 41-42 42-43 42-44 43-46 44-45 44-56 45-46
45-59 46-48
52-53 53-54 54-55 56-57 57-58 58-59 60-61 61-62 62-63 64-65 65-66 66-67
68-69 69-70
70-71 72-73 73-74 74-75 76-77 77-78 78-79 80-81 81-82 82-83 86-87 86-91
87-88 88-89
89-90 90-91

exact/norm bonds :

1-2 1-5 1-23 2-3 2-83 3-4 3-80 4-5 4-6 6-7 7-8 7-9 8-11 9-10 9-71
10-11 10-68 11-24 12-13 12-16 12-23 13-14 13-76 14-15 14-79 15-16 15-17
16-51 17-18 18-19
18-20 19-22 20-21 20-72 21-22 21-75 22-24 25-26 25-29 25-47 26-27 26-67
27-28 27-64
28-29 28-30 30-31 31-32 31-33 32-35 33-34 33-55 34-35 34-52 35-48 36-37
36-40 36-47
37-38 37-60 38-39 38-63 39-40 39-41 41-42 42-43 42-44 43-46 43-49 44-45
44-56 45-46
45-59 46-48 49-50 50-51 52-53 53-54 54-55 56-57 57-58 58-59 60-61 61-62
62-63 64-65
65-66 66-67 68-69 69-70 70-71 72-73 73-74 74-75 76-77 77-78 78-79 80-81
81-82 82-83
84-85 90-92 94-95 94-96 94-109 101-102 101-103 104-105 104-106

normalized bonds :

86-87 86-91 87-88 88-89 89-90 90-91

G1:X,Ak,CN,NO2,N,[*1],[*2],[*3],[*4],[*5],[*6]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom
22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom
31:Atom 32:Atom
33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom
42:Atom 43:Atom
44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:CLASS 50:CLASS 51:CLASS 52:Atom
53:Atom 54:Atom
55:Atom 56:Atom 57:Atom 58:Atom 59:Atom 60:Atom 61:Atom 62:Atom 63:Atom
64:Atom 65:Atom
66:Atom 67:Atom 68:Atom 69:Atom 70:Atom 71:Atom 72:Atom 73:Atom 74:Atom
75:Atom 76:Atom
77:Atom 78:Atom 79:Atom 80:Atom 81:Atom 82:Atom 83:Atom 84:CLASS 85:CLASS
86:Atom 87:Atom
88:Atom 89:Atom 90:Atom 91:Atom 92:CLASS 93:Atom 94:CLASS 95:CLASS 96:CLASS
101:CLASS
102:CLASS 103:CLASS 104:CLASS 105:CLASS 106:CLASS 109:CLASS 112:CLASS

10/516884

Generic attributes :

93:

Saturation : Unsaturated

```
L34      154 SEA FILE=REGISTRY SUB=L5 SSS FUL L32
L40      1 SEA FILE=REGISTRY ABB=ON PLU=ON L17 AND HYDROXIDE/CNS
L41      6 SEA FILE=REGISTRY ABB=ON PLU=ON L34 AND HYDROXIDE/CNS
L42      1 SEA FILE=REGISTRY ABB=ON PLU=ON L34 AND SULFATE/CNS
L44      154 SEA FILE=REGISTRY ABB=ON PLU=ON L17 OR L34
L46      7 SEA FILE=REGISTRY ABB=ON PLU=ON (L40 OR L41 OR L42)
L50      5 SEA FILE=ZCAPLUS ABB=ON PLU=ON L46
L57      1 SEA FILE=REGISTRY ABB=ON PLU=ON HYDROXIDE/CN
L58      1 SEA FILE=REGISTRY ABB=ON PLU=ON SULFATE/CN
L59      1 SEA FILE=REGISTRY ABB=ON PLU=ON CHLORIDE/CN
L60      0 SEA FILE=REGISTRY ABB=ON PLU=ON H S O/ELF
L61      30961 SEA FILE=REGISTRY ABB=ON PLU=ON H O S/ELF
L62      30964 SEA FILE=REGISTRY ABB=ON PLU=ON (L57 OR L58 OR L59 OR L60 OR
        L61)
L63      83 SEA FILE=ZCAPLUS ABB=ON PLU=ON L44
L64      50 SEA FILE=ZCAPLUS ABB=ON PLU=ON L17
L65      4 SEA FILE=ZCAPLUS ABB=ON PLU=ON L62 AND (L63 OR L64)
L66      4 SEA FILE=ZCAPLUS ABB=ON PLU=ON L65 NOT L50
L67      1 SEA FILE=ZCAPLUS ABB=ON PLU=ON L66 AND SULFATE/OBI
```

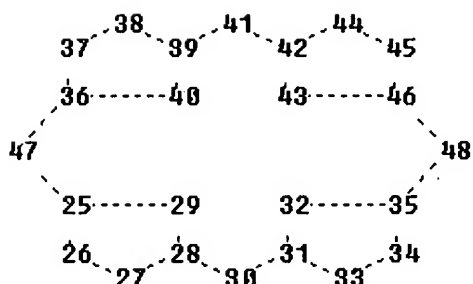
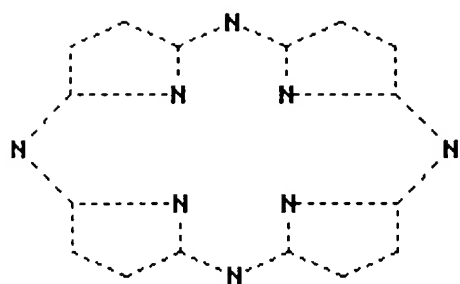
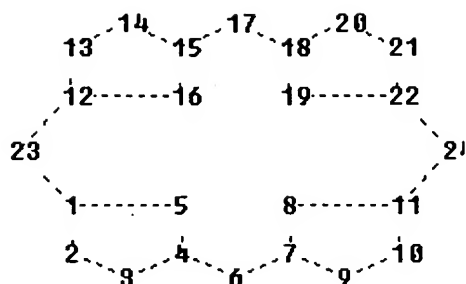
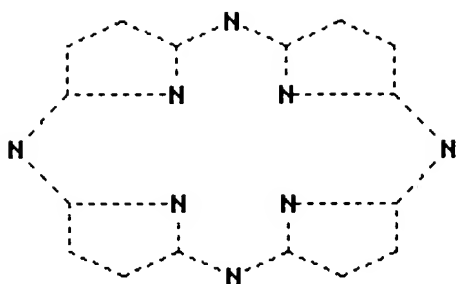
=> d stat que L69

L4 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:

Uploading L4b.str



ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44
45 46 47 48

ring bonds :

1-2 1-5 1-23 2-3 3-4 4-5 4-6 6-7 7-8 7-9 8-11 9-10 10-11 11-24 12-13
12-16 12-23 13-14 14-15 15-16 15-17 17-18 18-19 18-20 19-22 20-21 21-22
22-24 25-26
25-29 25-47 26-27 27-28 28-29 28-30 30-31 31-32 31-33 32-35 33-34 34-35
35-48 36-37
36-40 36-47 37-38 38-39 39-40 39-41 41-42 42-43 42-44 43-46 44-45 45-46
46-48

exact/norm bonds :

1-2 1-5 1-23 2-3 3-4 4-5 4-6 6-7 7-8 7-9 8-11 9-10 10-11 11-24 12-13
12-16 12-23 13-14 14-15 15-16 15-17 17-18 18-19 18-20 19-22 20-21 21-22
22-24 25-26
25-29 25-47 26-27 27-28 28-29 28-30 30-31 31-32 31-33 32-35 33-34 34-35
35-48 36-37
36-40 36-47 37-38 38-39 39-40 39-41 41-42 42-43 42-44 43-46 44-45 45-46
46-48

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom
22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom
31:Atom 32:Atom
33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom

10/516884

42:Atom 43:Atom

44:Atom 45:Atom 46:Atom 47:Atom 48:Atom

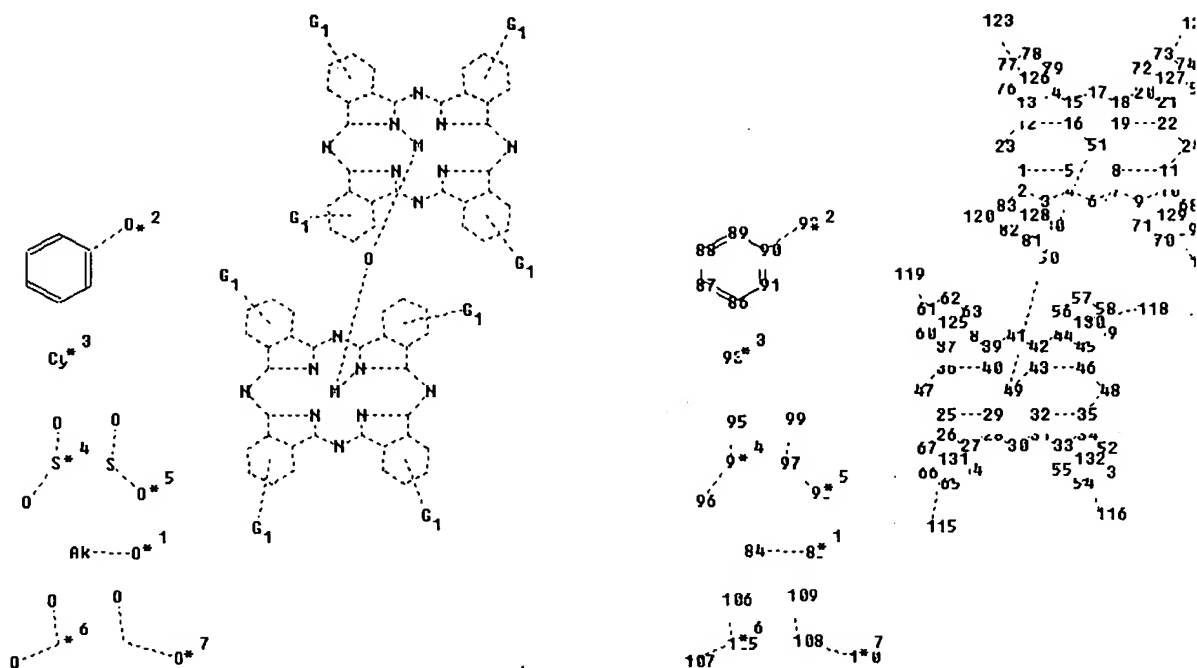
L5 2661 SEA FILE=REGISTRY SSS FUL L4

L15 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:

Uploading L15b.str



10/516884

ring bonds :

1-2	1-5	1-23	2-3	2-83	3-4	3-80	4-5	4-6	6-7	7-8	7-9	8-11	9-10	9-71
10-11	10-68	11-24	12-13	12-16	12-23	13-14	13-76	14-15	14-79	15-16	15-17			
17-18	18-19	18-20												
19-22	20-21	20-72	21-22	21-75	22-24	25-26	25-29	25-47	26-27	26-67	27-28			
27-64	28-29													
28-30	30-31	31-32	31-33	32-35	33-34	33-55	34-35	34-52	35-48	36-37	36-40			
36-47	37-38													
37-60	38-39	38-63	39-40	39-41	41-42	42-43	42-44	43-46	44-45	44-56	45-46			
45-59	46-48													
52-53	53-54	54-55	56-57	57-58	58-59	60-61	61-62	62-63	64-65	65-66	66-67			
68-69	69-70													
70-71	72-73	73-74	74-75	76-77	77-78	78-79	80-81	81-82	82-83	86-87	86-91			
87-88	88-89													
89-90	90-91													

exact/norm bonds :

1-2	1-5	1-23	2-3	2-83	3-4	3-80	4-5	4-6	6-7	7-8	7-9	8-11	9-10	9-71
10-11	10-68	11-24	12-13	12-16	12-23	13-14	13-76	14-15	14-79	15-16	15-17			
16-51	17-18	18-19												
18-20	19-22	20-21	20-72	21-22	21-75	22-24	25-26	25-29	25-47	26-27	26-67			
27-28	27-64													
28-29	28-30	30-31	31-32	31-33	32-35	33-34	33-55	34-35	34-52	35-48	36-37			
36-40	36-47													
37-38	37-60	38-39	38-63	39-40	39-41	41-42	42-43	42-44	43-46	43-49	44-45			
44-56	45-46													
45-59	46-48	49-50	50-51	52-53	53-54	54-55	56-57	57-58	58-59	60-61	61-62			
62-63	64-65													
65-66	66-67	68-69	69-70	70-71	72-73	73-74	74-75	76-77	77-78	78-79	80-81			
81-82	82-83													
84-85	90-92	94-95	94-96	97-98	97-99	105-106	105-107	108-109	108-110					

normalized bonds :

86-87	86-91	87-88	88-89	89-90	90-91
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G1:N,CN,NO2,X,Ak, [*1], [*2], [*3], [*4], [*5], [*6], [*7]

Match level :

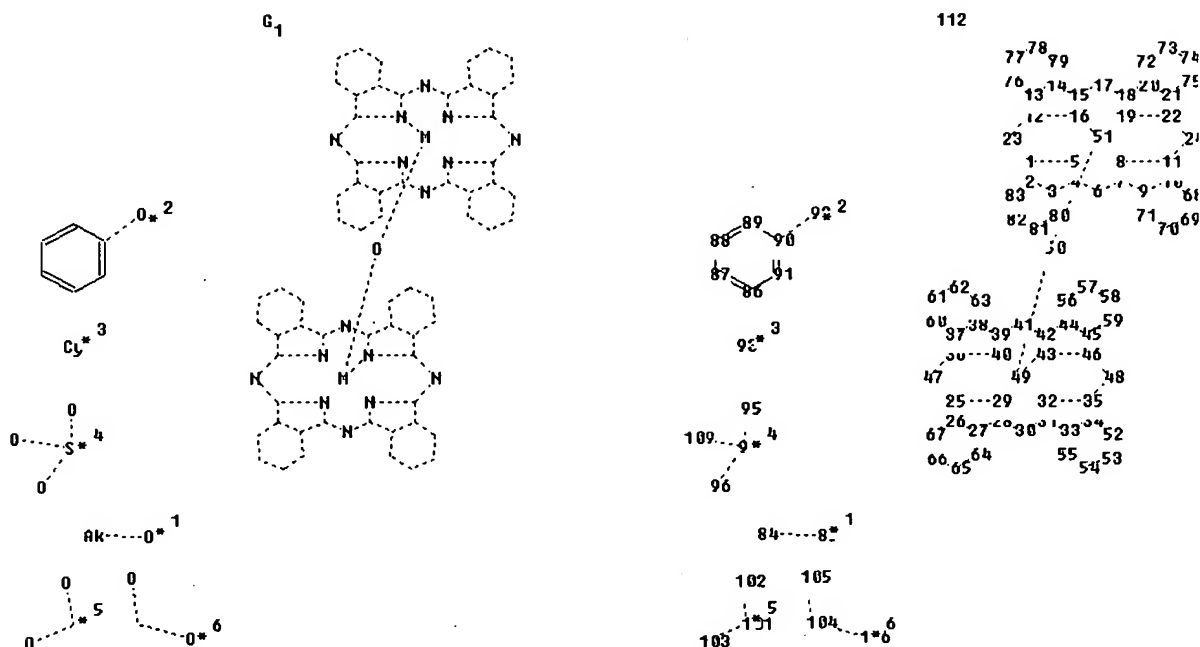
1:Atom	2:Atom	3:Atom	4:Atom	5:Atom	6:Atom	7:Atom	8:Atom	9:Atom	10:Atom
11:Atom	12:Atom	13:Atom	14:Atom	15:Atom	16:Atom	17:Atom	18:Atom	19:Atom	
20:Atom	21:Atom								
22:Atom	23:Atom	24:Atom	25:Atom	26:Atom	27:Atom	28:Atom	29:Atom	30:Atom	
31:Atom	32:Atom								
33:Atom	34:Atom	35:Atom	36:Atom	37:Atom	38:Atom	39:Atom	40:Atom	41:Atom	
42:Atom	43:Atom								
44:Atom	45:Atom	46:Atom	47:Atom	48:Atom	49:CLASS	50:CLASS	51:CLASS	52:Atom	
53:Atom	54:Atom								
55:Atom	56:Atom	57:Atom	58:Atom	59:Atom	60:Atom	61:Atom	62:Atom	63:Atom	
64:Atom	65:Atom								
66:Atom	67:Atom	68:Atom	69:Atom	70:Atom	71:Atom	72:Atom	73:Atom	74:Atom	
75:Atom	76:Atom								
77:Atom	78:Atom	79:Atom	80:Atom	81:Atom	82:Atom	83:Atom	84:CLASS	85:CLASS	
86:Atom	87:Atom								
88:Atom	89:Atom	90:Atom	91:Atom	92:CLASS	93:Atom	94:CLASS	95:CLASS	96:CLASS	
97:CLASS									
98:CLASS	99:CLASS	105:CLASS	106:CLASS	107:CLASS	108:CLASS	109:CLASS			
110:CLASS	115:CLASS	116:CLASS							
118:CLASS	119:CLASS	120:CLASS	121:CLASS	122:CLASS	123:CLASS	125:Atom			
126:Atom	127:Atom								
128:Atom	129:Atom	130:Atom	131:Atom	132:Atom					

Generic attributes :

Saturation : Unsaturated

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:
Uploading L32b.str



33

10/516884

ring bonds :

1-2 1-5 1-23 2-3 2-83 3-4 3-80 4-5 4-6 6-7 7-8 7-9 8-11 9-10 9-71
10-11 10-68 11-24 12-13 12-16 12-23 13-14 13-76 14-15 14-79 15-16 15-17
17-18 18-19 18-20
19-22 20-21 20-72 21-22 21-75 22-24 25-26 25-29 25-47 26-27 26-67 27-28
27-64 28-29
28-30 30-31 31-32 31-33 32-35 33-34 33-55 34-35 34-52 35-48 36-37 36-40
36-47 37-38
37-60 38-39 38-63 39-40 39-41 41-42 42-43 42-44 43-46 44-45 44-56 45-46
45-59 46-48
52-53 53-54 54-55 56-57 57-58 58-59 60-61 61-62 62-63 64-65 65-66 66-67
68-69 69-70
70-71 72-73 73-74 74-75 76-77 77-78 78-79 80-81 81-82 82-83 86-87 86-91
87-88 88-89
89-90 90-91

exact/norm bonds :

1-2 1-5 1-23 2-3 2-83 3-4 3-80 4-5 4-6 6-7 7-8 7-9 8-11 9-10 9-71
10-11 10-68 11-24 12-13 12-16 12-23 13-14 13-76 14-15 14-79 15-16 15-17
16-51 17-18 18-19
18-20 19-22 20-21 20-72 21-22 21-75 22-24 25-26 25-29 25-47 26-27 26-67
27-28 27-64
28-29 28-30 30-31 31-32 31-33 32-35 33-34 33-55 34-35 34-52 35-48 36-37
36-40 36-47
37-38 37-60 38-39 38-63 39-40 39-41 41-42 42-43 42-44 43-46 43-49 44-45
44-56 45-46
45-59 46-48 49-50 50-51 52-53 53-54 54-55 56-57 57-58 58-59 60-61 61-62
62-63 64-65
65-66 66-67 68-69 69-70 70-71 72-73 73-74 74-75 76-77 77-78 78-79 80-81
81-82 82-83
84-85 90-92 94-95 94-96 94-109 101-102 101-103 104-105 104-106

normalized bonds :

86-87 86-91 87-88 88-89 89-90 90-91

G1:X,Ak,CN,NO2,N,[*1],[*2],[*3],[*4],[*5],[*6]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom
22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom
31:Atom 32:Atom
33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom
42:Atom 43:Atom
44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:CLASS 50:CLASS 51:CLASS 52:Atom
53:Atom 54:Atom
55:Atom 56:Atom 57:Atom 58:Atom 59:Atom 60:Atom 61:Atom 62:Atom 63:Atom
64:Atom 65:Atom
66:Atom 67:Atom 68:Atom 69:Atom 70:Atom 71:Atom 72:Atom 73:Atom 74:Atom
75:Atom 76:Atom
77:Atom 78:Atom 79:Atom 80:Atom 81:Atom 82:Atom 83:Atom 84:CLASS 85:CLASS
86:Atom 87:Atom
88:Atom 89:Atom 90:Atom 91:Atom 92:CLASS 93:Atom 94:CLASS 95:CLASS 96:CLASS
101:CLASS
102:CLASS 103:CLASS 104:CLASS 105:CLASS 106:CLASS 109:CLASS 112:CLASS

Generic attributes :

93:

Saturation : Unsaturated

L34 154 SEA FILE=REGISTRY SUB=L5 SSS FUL L32
 L44 154 SEA FILE=REGISTRY ABB=ON PLU=ON L17 OR L34
 L63 83 SEA FILE=ZCAPLUS ABB=ON PLU=ON L44
 L64 50 SEA FILE=ZCAPLUS ABB=ON PLU=ON L17
 L68 581403 SEA FILE=ZCAPLUS ABB=ON PLU=ON CHARGE/BI
 L69 8 SEA FILE=ZCAPLUS ABB=ON PLU=ON (L63 OR L64) AND L68

=> s (L38 or L50 or L67 or L69) not (L72 or L73)
 L75 9 (L38 OR L50 OR L67 OR L69) NOT (L72 OR L73)

=> d ibib abs hitind hitstr L75 1-9

L75 ANSWER 1 OF 9 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:981679 ZCAPLUS Full-text

DOCUMENT NUMBER: 143:485704

TITLE: Photoredox reaction of (Pcts)FeIII(O22-)FeIII(Pcts) with PctsH2 = phthalocyaninetetrasulfonate induced by peroxide to Fe(III) **charge** transfer excitation

AUTHOR(S): Kunkely, Horst; Vogler, Arnd

CORPORATE SOURCE: Institut fuer Anorganische Chemie, Universitaet Regensburg, Regensburg, D-93040, Germany

SOURCE: Inorganica Chimica Acta (2005), 358(13), 4086-4088
 CODEN: ICHAA3; ISSN: 0020-1693

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The binuclear complex (Pcts)FeIII(O22-)FeIII(Pcts) where PctsH = phthalocyaninetetrasulfonate is stable in aqueous solution for some time (.apprx.1 h) before it is irreversibly converted to (Pcts)FeIII-O-FeIII(Pcts). The photolysis of the peroxo complex in argon-saturated water leads to the release of oxygen and the formation of FeII(Pcts) with .vphi. = 5 + 10-4 at $\lambda_{irr} = 333$ nm. It is suggested that this photoredox reaction originates from a peroxide to FeIII LMCT state. It is populated from Pcts IL states which are initially reached by light absorption.

CC 74-1 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)

IT **Charge** transfer transition

(ligand-to-metal; photolysis of binuclear iron phthalocyaninetetrasulfonate peroxo complex in argon-saturated aqueous solution)

IT 7782-44-7P, Oxygen, properties **721882-48-0P**

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (photoproduct; photolysis of binuclear iron phthalocyaninetetrasulfonate peroxo complex in argon-saturated aqueous solution)

IT **721882-48-0P**

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (photoproduct; photolysis of binuclear iron phthalocyaninetetrasulfonate peroxo complex in argon-saturated aqueous solution)

RN 721882-48-0 ZCAPLUS

CN Ferrate(8-), μ -oxobis[29H,31H-phthalocyanine-2,9,16,23-tetrasulfonato(6-)- κ N29, κ N30, κ N31, κ N32]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L75 ANSWER 2 OF 9 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1998:392995 ZCAPLUS Full-text

DOCUMENT NUMBER: 129:141830

TITLE: Anodic oxidation of cysteine catalyzed by nickel
tetrasulfonated phthalocyanine immobilized on silica
gel modified with titanium(IV) oxide

AUTHOR(S): Perez, Elizabeth F.; Kubota, Lauro T.; Tanaka, Auro
A.; De Oliveira Neto, Graciliano

CORPORATE SOURCE: Instituto de Quimica, UNICAMP, Campinas, 13083-970,
Brazil

SOURCE: Electrochimica Acta (1998), 43(12-13), 1665-1673
CODEN: ELCAAV; ISSN: 0013-4686

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A chemical modified electrode constructed by mixing nickel tetrasulfonated
phthalocyanine (NiTsPc) immobilized on modified silica gel with carbon paste
showed a redox process with a midpoint potential of 0.44 V vs. SCE. Expts.
carried out with different supporting electrolytes suggested an effect due to
the nature of the anion. The solution pH does not affect the midpoint
potential but the peak current increases when the pH is decreased. The
immobilization procedure causes an increase in the monomeric form of the
complex. The electrochem. property of NiTsPc adsorbed onto modified silica
showed good stability even in acidic media (pH = 2) and the ability to
catalyze the electrooxidn. of cysteine at 0.5 V vs. SCE.

CC 72-2 (Electrochemistry)

Section cross-reference(s): 22, 66, 67, 78

IT 210690-34-9 210690-35-0

RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation,
nonpreparative)

(effect of nitrogen or oxygen or air on Ni tetrasulfonated
phthalocyanine dimer formation in aqueous solution: electrooxidn. of
cysteine

catalyzed by Ni tetrasulfonated phthalocyanine immobilized on silica
gel modified with Ti(IV) oxide)

IT 71-50-1, Acetic acid, ion(1-), uses 14127-61-8, Calcium(2+), uses
14797-55-8, Nitrate, uses 14797-73-0, Perchlorate 14798-03-9,
Ammonium, uses 14808-79-8, Sulfate, uses

16887-00-6, Chloride, uses 17341-24-1, Lithium(1+), uses

17341-25-2, Sodium(1+), uses 24203-36-9, Potassium(1+), uses

RL: NUU (Other use, unclassified); PRP (Properties); USES (Uses)

(midpoint potential for nickel tetrasulfonated phthalocyanine
immobilized on silica gel modified with titanium(IV) oxide in solution
containing)

IT 210690-34-9

RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation,
nonpreparative)

(effect of nitrogen or oxygen or air on Ni tetrasulfonated
phthalocyanine dimer formation in aqueous solution: electrooxidn. of
cysteine

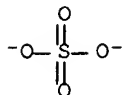
catalyzed by Ni tetrasulfonated phthalocyanine immobilized on silica
gel modified with Ti(IV) oxide)

RN 210690-34-9 ZCAPLUS

CN Nickelate(10-), μ -oxobis[29H,31H-phthalocyanine-2,9,16,23-
tetrasulfonato(6-)- κ N29, κ N30, κ N31, κ N32]di- (9CI)
(CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

IT 14808-79-8, Sulfate, uses 16887-00-6,
Chloride, uses
RL: NUU (Other use, unclassified); PRP (Properties); USES (Uses)
(midpoint potential for nickel tetrasulfonated phthalocyanine
immobilized on silica gel modified with titanium(IV) oxide in solution
containing)
RN 14808-79-8 ZCAPLUS
CN Sulfate (7CI, 8CI, 9CI) (CA INDEX NAME)



RN 16887-00-6 ZCAPLUS
CN Chloride (CA INDEX NAME)

Cl-

REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L75 ANSWER 3 OF 9 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:81051 ZCAPLUS Full-text
DOCUMENT NUMBER: 124:218437
TITLE: Interaction of manganese phthalocyanine with
tetracyanoquinodimethane in solution
AUTHOR(S): Sidorov, A. N.
CORPORATE SOURCE: Vavilov State Optical Inst., All-Russia Scientific
Center, St. Petersburg, 193171, Russia
SOURCE: Russian Journal of Coordination Chemistry (Translation
of Koordinatsionnaya Khimiya) (1995), 21(12), 898-900
CODEN: RJCCEY; ISSN: 1070-3284
PUBLISHER: MAIK Nauka/Interperiodica
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The interaction between the Mn(II) phthalocyanine complex (MnPc) and
tetracyanoquinodimethane (TCNQ) in a solution of a THF-Et₂O mixture was
studied by electronic absorption spectroscopy. The interaction has the donor-
acceptor nature, with the Mn atom as a donor. It is assumed that the reaction
product has the MnIIIPc(TCNQ)- structure. The reaction of TCNQ with oxidized
MnPc yields the **charge**-transfer complex (TCNQ) δ^- ·PcMnIII-O-MnIIIPc·(TCNQ) δ^- .
The Zn and Fe phthalocyanine complexes and the Lu diphtalocyanine complex do
not react with TCNQ.
CC 78-3 (Inorganic Chemicals and Reactions)
ST manganese phthalocyanine TCNQ **charge** transfer complex
IT Electron exchange and **Charge** transfer
(manganese phthalocyanine TCNQ complexes)
IT 174582-02-6 174582-03-7

10/516884

RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(formation and absorption spectra of)

IT 174582-03-7

RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(formation and absorption spectra of)

RN 174582-03-7 ZCAPLUS

CN Manganese, bis[2,2'-(2,5-cyclohexadiene-1,4-diylidene)bis[propanedinitrile]-N]-μ-oxobis[29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]di- (9CI)
(CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L75 ANSWER 4 OF 9 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1994:148867 ZCAPLUS Full-text

DOCUMENT NUMBER: 120:148867

TITLE: High-photosensitivity electrophotographic photoreceptor

INVENTOR(S): Tai, Seiji; Katayose, Mitsuo; Morishita, Yoshii

PATENT ASSIGNEE(S): Hitachi Chemical Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 22 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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JP 04362653	A	19921215	JP 1991-138909	19910611
PRIORITY APPLN. INFO.:			JP 1991-138909	19910611

GI For diagram(s), see printed CA Issue.

AB In the title electrophotog. photoreceptor comprising an organic photoconductive layer on an elec. conductive support, I [M = Al, Ga, In, Si, Ge, Sn; Al-8 = benzene ring, naphthalene ring, anthracene ring, N-containing aromatic ring; X = halo, R1, OR2, SR3, SiR4R5R6, SO2NR7R8, SO2R9, COR10, COOR11, CONHR12, NR13R14, R15OR16, NO2, SO3H, CN, NHCOR17; g, h, i, j, k, l, m, n = 0-8; Y1,2 = halo, OH, R18, OR19, OSiR20R21R22; R1-22 = H, alkyl, cycloalkyl, aryl, halogenated alkyl, Si-containing group] is utilized as a photoconductive substance in the photoconductive layer. The photoreceptor shows high photosensitivity to the long wavelength region and is suitable for use in a laser printer.

IC ICM G03G005-06

CC 74-3 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)

ST electrophotog photoreceptor **charge** generating substance

IT Electrophotographic photoconductors and photoreceptors
(**charge**-generating substances for)

IT 151629-23-1 151629-24-2 151896-69-4 151987-51-8 151987-55-2
151989-12-7 151989-13-8 151989-14-9 151989-15-0
151989-16-1 151989-18-3 151989-19-4 151989-20-7
151989-21-8 151989-22-9 151989-23-0 151989-24-1
151989-25-2 152014-43-2 153244-87-2

RL: USES (Uses)

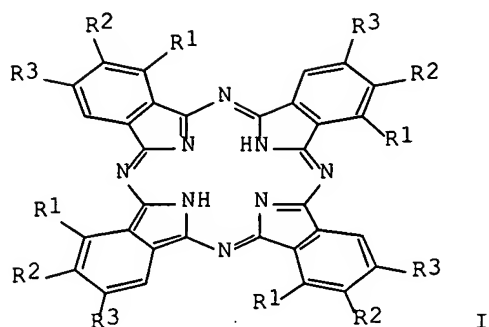
(**charge**-generating material, for electrophotog. photoreceptor)

IT 151627-42-8D, derivs.

RL: USES (Uses)

(**charge**-generating materials, for electrophotog.)

photoreceptors)
 IT 151627-42-8P 151987-52-9P 151987-53-0P 151987-54-1P 151989-17-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and use of, as **charge**-generating material, for
 electrophotog. photoreceptor)
 IT 995-25-5, Tri(propyl)chlorosilane 3468-11-9 13134-31-1,
 2,3-Diaminopyrazine 19333-10-9, Dichlorosilicon phthalocyanine
 82039-07-4, Boron tetrachloride 127009-68-1 151629-11-7 151871-31-7
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, **charge**-generating material from, for
 electrophotog. photoreceptor)
 IT 151989-13-8 151989-14-9 151989-19-4
 151989-21-8 151989-25-2
 RL: USES (Uses)
 (**charge**-generating material, for electrophotog.
 photoreceptor)
 RN 151989-13-8 ZCAPLUS
 CN Gallium, μ -oxobis[C,C,C,C-tetrabromo-29H,31H-phthalocyaninato(2-)-
 N29,N30,N31,N32]di- (9CI) (CA INDEX NAME)
 *** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
 RN 151989-14-9 ZCAPLUS
 CN Indium, μ -oxobis[C,C,C,C-tetranitro-29H,31H-phthalocyaninato(2-)-
 N29,N30,N31,N32]di- (9CI) (CA INDEX NAME)
 *** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
 RN 151989-19-4 ZCAPLUS
 CN Germanium, μ -oxobis[29H,31H-phthalocyanine-C,C,C,C-tetrasulfonamidato(2-)-
 N29,N30,N31,N32]bis(tripropylsilanolato)di- (9CI) (CA INDEX NAME)
 *** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
 RN 151989-21-8 ZCAPLUS
 CN Tin, μ -oxo[C,C,C,C-tetrakis(methylsulfonyl)-29H,31H-phthalocyaninato(2-)-
 N29,N30,N31,N32][C,C,C,C-tetrakis(methylsulfonyl)-37H,39H-
 tetranaphtho[2,3-b:2',3'-g:2'',3''-l:2''',3'''-q]porphyrizinato(2-)-
 N37,N38,N39,N40]bis(tripropylsilanolato)di- (9CI) (CA INDEX NAME)
 *** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
 RN 151989-25-2 ZCAPLUS
 CN Germanium, μ -oxobis[tetramethyl 37H,39H-tetranaphtho[2,3-b:2',3'-
 g:2'',3''-l:2''',3'''-q]porphyrazine-C,C,C,C-tetracarboxylato(2-)-
 N37,N38,N39,N40]bis(tripropylsilanolato)di- (9CI) (CA INDEX NAME)
 *** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
 L75 ANSWER 5 OF 9 ZCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1993:572853 ZCAPLUS Full-text
 DOCUMENT NUMBER: 119:172853
 TITLE: Phthalocyanines and related compounds. XXXV. Synthesis
 and coordination chemistry of substituted manganese
 phthalocyanines
 AUTHOR(S): Dolotova, O. V.; Bundina, N. I.; Derkacheva, V. M.;
 Negrimovskii, V. M.; Minin, V. V.; Larin, G. M.;
 Kaliya, O. L.; Luk'yanets, E. A.
 CORPORATE SOURCE: NII Org. Poluprod. Krasitel., Moscow, Russia
 SOURCE: Zhurnal Obshchei Khimii (1992), 62(9), 2064-75
 CODEN: ZOKHA4; ISSN: 0044-460X
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian



AB Reaction of substituted phthalonitriles and $\text{Mn}(\text{OAc})_2$ in the presence of $(\text{NH}_4)_2\text{MoO}_4$ gave MnLX ($\text{H}_2\text{L} = \text{I}$ ($\text{R}_1 = \text{R}_3 = \text{H}$, $\text{R}_2 = \text{Me}_3\text{C}$, PhSO_3 , Me_3CO , Me_3CS , piperidine; $\text{R}_2 = \text{R}_3 = \text{H}$, $\text{R}_1 = \text{o-ClC}_6\text{H}_4$, PhSO_2 , PhS ; $\text{R}_2 = \text{H}$, $\text{R}_3 = \text{Me}_3\text{C}$, $\text{R}_1 = \text{PhSO}_2$, PhS , Me_2N or $\text{R}_3 = \text{R}_1 = \text{NO}_2$, PhSO_2); $\text{X} = \text{Cl}$, OH , OAc). MnLX in pyridine reacted with hot H_2O to give $[(\text{py})\text{LMn}]_{20}$. MnL were obtained by reaction of MnLX with KOH under anaerobic conditions. In pyridine MnL form $\text{MnL}(\text{py})_n$ ($n = 1, 2$) according to electronic spectra. Their stability toward oxidation-reduction and protolytic conversion depends on the nature of the substituents. Possible electronic isomers of $\text{LMnII}(\text{py})_n$ (MnIII and MnI **charge** transfer compds.) are discussed and these are explained by the energetic nearness of the d-orbitals of Mn and the π -orbitals of L.

CC 78-7 (Inorganic Chemicals and Reactions)

Section cross-reference(s): 26

ST manganese phthalocyaninato complex; **charge** transfer manganese phthalocyaninato complex

IT 117778-18-4P 117778-20-8P 117778-21-9P 117778-22-0P 117778-23-1P
 117778-24-2P 149785-81-9P 149785-82-0P 149785-83-1P 149785-84-2P
 149785-85-3P 149785-86-4P 149785-87-5P 149785-88-6P 149785-89-7P
 149785-90-0P 149785-91-1P 149785-92-2P 149785-93-3P 149785-94-4P
 149785-95-5P 149785-96-6P 149785-97-7P 149785-98-8P 149785-99-9P
 149786-00-5P 149786-01-6P 149786-02-7P 149786-03-8P
149825-79-6P 149825-80-9P 149825-81-0P
 149855-30-1P 149855-31-2P 149855-32-3P 149855-33-4P 149855-34-5P
 149855-35-6P 149855-36-7P **149855-37-8P 149855-38-9P**
149855-39-0P 149855-40-3P 149855-41-4P
149855-42-5P 149855-43-6P 149855-44-7P
149855-45-8P 149855-46-9P 149855-47-0P 150120-75-5P

RL: PRP (Properties); PREP (Preparation)

(formation and visible spectrum of)

IT **149825-82-1P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

IT **149825-79-6P 149825-80-9P 149825-81-0P**
149855-37-8P 149855-38-9P 149855-39-0P
149855-40-3P 149855-41-4P 149855-42-5P
149855-43-6P 149855-44-7P 149855-45-8P
 RL: PRP (Properties); PREP (Preparation)
 (formation and visible spectrum of)

10/516884

RN 149825-79-6 ZCAPLUS

CN Manganese, μ -oxobis(pyridine)bis[3,10,17,24-tetrakis(1,1-dimethylethyl)-N,N,N',N',N'',N'',N''',N''''-octamethyl-29H,31H-phthalocyanine-1,8,15,22-tetraminato(2-)-N29,N30,N31,N32]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 149825-80-9 ZCAPLUS

CN Manganese, bis[1,3,8,10,15,17,22,24-octanitro-29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]- μ -oxobis(pyridine)di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 149825-81-0 ZCAPLUS

CN Manganese, bis[1,3,8,10,15,17,22,24-octakis(phenylsulfonyl)-29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]- μ -oxobis(pyridine)di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 149855-37-8 ZCAPLUS

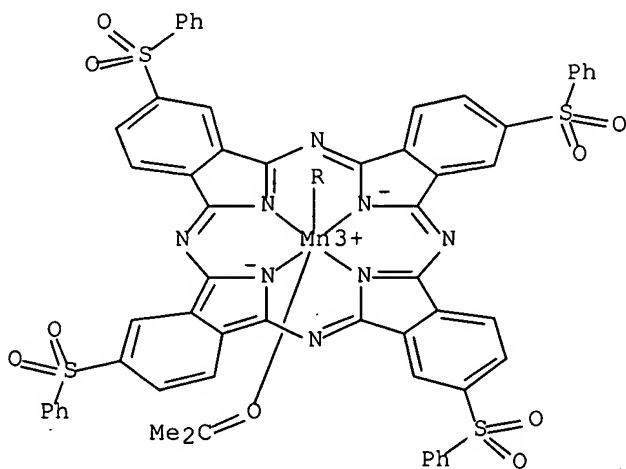
CN Manganese, μ -oxobis(pyridine)bis[2,9,16,23-tetrakis(1,1-dimethylethyl)-29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]di- (9CI) (CA INDEX NAME)

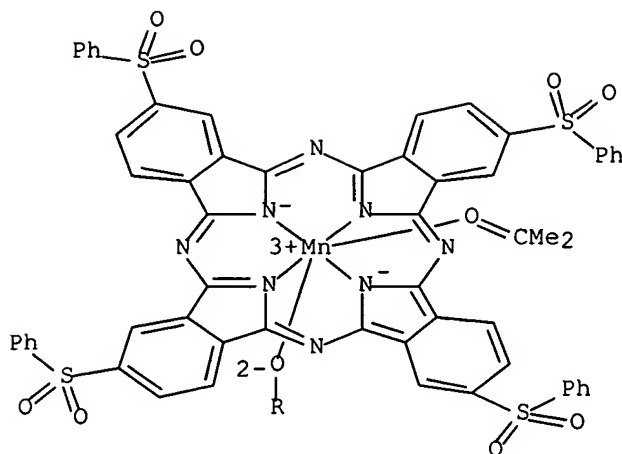
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 149855-38-9 ZCAPLUS

CN Manganese, μ -oxobis(2-propanone)bis[2,9,16,23-tetrakis(phenylsulfonyl)-29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]di- (9CI) (CA INDEX NAME)

PAGE 1-A





RN 149855-39-0 ZCAPLUS

CN Manganese, μ -oxobis(pyridine)bis[2,9,16,23-tetrakis(1,1-dimethylethoxy)-29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 149855-40-3 ZCAPLUS

CN Manganese, μ -oxobis(pyridine)bis[2,9,16,23-tetrakis[(1,1-dimethylethyl)thio]-29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 149855-41-4 ZCAPLUS

CN Manganese, μ -oxobis(pyridine)bis[2,9,16,23-tetra-1-piperidinyl-29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 149855-42-5 ZCAPLUS

CN Manganese, μ -oxobis(pyridine)bis[1,8,15,22-tetrakis(phenylsulfonyl)-29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 149855-43-6 ZCAPLUS

CN Manganese, μ -oxobis(pyridine)bis[1,8,15,22-tetrakis(phenylthio)-29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 149855-44-7 ZCAPLUS

CN Manganese, μ -oxobis(pyridine)bis[3,10,17,24-tetrakis(1,1-dimethylethyl)-1,8,15,22-tetrakis(phenylsulfonyl)-29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 149855-45-8 ZCAPLUS

CN Manganese, μ -oxobis(pyridine)bis[3,10,17,24-tetrakis(1,1-dimethylethyl)-1,8,15,22-tetrakis(phenylthio)-29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

10/516884

IT 149825-82-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 149825-82-1 ZCAPLUS

CN Manganese, diaqua- μ -oxobis[2,9,16,23-tetrakis(phenylsulfonyl)-29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L75 ANSWER 6 OF 9 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1992:70397 ZCAPLUS Full-text

DOCUMENT NUMBER: 116:70397

TITLE: Studies of the adsorption of tetrasulfonated
phthalocyanines on graphite substrate

AUTHOR(S): Gupta, S.; Huang, H.; Yeager, E.

CORPORATE SOURCE: Case Cent. Electrochem. Sci., Case West. Reserve
Univ., Cleveland, OH, 44106, USA

SOURCE: Electrochimica Acta (1991), 36(14), 2165-9

CODEN: ELCAAV; ISSN: 0013-4686

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The adsorption of iron and cobalt tetrasulfonated phthalocyanines (FeTsPc and CoTsPc, resp.) on ordinary pyrolytic graphite was investigated as a function of pH and ionic strength of the adsorption solution as well as the potential. The **charge** corresponding to the voltammetric redox peaks of adsorbed complexes was used as a measure of the surface concentration. Adsorption of CoTsPc occurs readily from its freshly prepared aqueous solns. and is generally independent of pH. For FeTsPc, however, adsorption does strongly depend on pH. High surface coverage is achieved only from acid solns. rather than from pure water and alkaline solns. This can be explained in terms of the form(s) of the complexes existing in the solution phase in the presence of air. UV-visible spectroscopic studies coupled with the addition of CN⁻ to the macrocycle solns. provide evidence that in pure water and alkaline solns. FeTsPc exists predominantly in the μ -oxo form (FeTsPc)₂O, which seems not to favor the adsorption process. No evidence of the μ -oxo complex was found for FeTsPc in acid solns. and CoTsPc in aqueous solns. over the pH range examined (1-13). The adsorption of FeTsPc was at maximum when the potential was held at -0.55 V vs. SCE in 0.1M NaOH.

CC 72-2 (Electrochemistry)

Section cross-reference(s): 66, 67

IT 138708-72-2P

RL: FORM (Formation, nonpreparative); PREP (Preparation)

(formation of, from monomer in alkaline solns., adsorption of monomer by
graphite electrode in relation to)

IT 138708-72-2P

RL: FORM (Formation, nonpreparative); PREP (Preparation)

(formation of, from monomer in alkaline solns., adsorption of monomer by
graphite electrode in relation to)

RN 138708-72-2 ZCAPLUS

CN Ferrate(8-), μ -oxobis[29H,31H-phthalocyanine-2,9,16,23-tetrasulfonato(6-)-N29,N30,N31,N32]di-, octahydrogen (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L75 ANSWER 7 OF 9 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1985:122955 ZCAPLUS Full-text

DOCUMENT NUMBER: 102:122955

TITLE: **Charge**-transfer and ligand-centered
photochemistry of manganese(III) phthalocyanines

10/516884

AUTHOR(S): Ferraudi, G.; Granifo, J.
CORPORATE SOURCE: Radiat. Lab., Univ. Notre Dame, Notre Dame, IN, 46556,
USA

SOURCE: Journal of Physical Chemistry (1985), 89(7), 1206-10
CODEN: JPCHAX; ISSN: 0022-3654

DOCUMENT TYPE: Journal
LANGUAGE: English

AB The UV photochem. of the Mn phthalocyanines, MnIII(tspc)(OH₂)(OH)₄⁻ and (H₂O)(tspc)MnIII-O-MnIII(tspc)(OH)₉⁻ (tspc = tetrasulfophthalocyanine) was investigated by continuous and flash photolysis. A significant **charge-transfer** photochem., namely, oxidation of the hydroxide or μ -oxo bridge and the reduction of the metal center was found with both complexes. In addition, the abstraction of H from appropriate donors by phthalocyanine centered $n\pi^*$ states was also detected. The fate of the Mn(II) species depends on the scavenger used for trapping HO \cdot radicals or reactive $n\pi^*$ states. So reactions of the 2-hydroxy-2-Pr, hydroxycyclohexadienyl, and hydroxycyclohexadienylsulfonate radicals with either Mn(II) or Mn(III) phthalocyanines determine the nature of the reaction products. The dependence of the rate of the μ -oxo dimer photodissocn. on light intensity demonstrated that recombination of the reduced and oxidized species limited the extent of the conversion to products. The relationship between the photochem. of the Mn(III) phthalocyanines and other metallophthalocyanines is discussed.

CC 74-1 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)

ST manganese phthalocyanine **charge** transfer photochem; photolysis
manganese sulfophthalocyanine

IT 12581-70-3

RL: RCT (Reactant); RACT (Reactant or reagent)
(photochem. of, **charge-transfer** and ligand centered)

IT 27288-51-3

RL: RCT (Reactant); RACT (Reactant or reagent)
(photochem. of, **charge-transfer** and ligand-centered)

IT 12581-70-3

RL: RCT (Reactant); RACT (Reactant or reagent)
(photochem. of, **charge-transfer** and ligand centered)

RN 12581-70-3 ZCAPLUS

CN Manganate(9-), aquahydroxy- μ -oxobis[29H,31H-phthalocyanine-C,C,C,C-tetrasulfonato(6-)-N29,N30,N31,N32]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L75 ANSWER 8 OF 9 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1976:83524 ZCAPLUS Full-text

DOCUMENT NUMBER: 84:83524

ORIGINAL REFERENCE NO.: 84:13619a,13622a

TITLE: Structure and properties of binuclear cobalt(IV)
phthalocyanine complexes

AUTHOR(S): Przywarska-Boniecka, Helena; Wojciechowski, Walter

CORPORATE SOURCE: Inst. Chem., Univ. Wroclaw, Wroclaw, Pol.

SOURCE: Materials Science (1975), 1(1), 27-35

CODEN: MSCJDS; ISSN: 0137-1339

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The complexes $[\{Co(H_2O)Pc\}_2SO_4]$, $[\{Co(OH)Pc\}_2O]$, $[\{Co(NH_3)Pc\}NH_2\{Co(H_2O)Pc\}]Cl_3$, $[\{Co(NH_3)Pc\}NH_2\{Co(NO_3)Pc\}]SO_4$, $[\{Co(NH_3)Pc\}O\{Co(OH)Pc\}]Cl$, and $[\{CoL(H_2O)\}OH\{CoL(OH)\}]SO_4$, where H₂Pc = phthalocyanine and H₂L = tetrasodium phthalocyaninetetrasulfonate, were prepared and characterized by magnetic susceptibility measurements and ESR, ir and electronic spectra.

10/516884

CC 78-7 (Inorganic Chemicals and Reactions)
IT 57756-66-8P 57756-67-9P 57756-69-1P 57756-73-7P
58098-47-8P 58343-92-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 57756-73-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 57756-73-7 ZCAPLUS
CN Cobaltate(6-), aqua- μ -hydroxyhydroxybis[29H,31H-phthalocyanine-C,C,C,C-
tetrasulfonato(6-)-N29,N30,N31,N32]di-, sodium sulfate (1:8:1) (9CI) (CA
INDEX NAME)

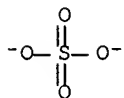
CM 1

CRN 57756-72-6
CMF C64 H28 Co2 N16 O27 S8
CCI CCS, IDS

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

CM 2

CRN 14808-79-8
CMF O4 S



L75 ANSWER 9 OF 9 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1976:11261 ZCAPLUS Full-text
DOCUMENT NUMBER: 84:11261
ORIGINAL REFERENCE NO.: 84:1801a,1804a
TITLE: Electric properties of some cobalt, chromium, and
manganese phthalocyanine complexes
AUTHOR(S): Makles, Monika; Przywarska-Bonieceka, Helena;
Wojciechowski, Walter
CORPORATE SOURCE: Inst. Chem., Univ. Wroclaw, Wroclaw, Pol.
SOURCE: Roczniki Chemii (1975), 49(10), 1647-53
CODEN: ROCHAC; ISSN: 0035-7677
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The elec. properties of 10 phthalocyanine compds. with Co, Cr, and Mn were
studied at 160-330°K. From elec.-conductivity measurements of polycryst.
samples of the complexes as a function of temperature, the activation energies
of conductivity were determined. Decreases of activation energy at certain
temps. indicated structural changes of the compds. In those regions, ionic
conductivity was observed. Low activation energies of the complexes containing
ions in the outer spheres may be accounted for by the contribution of the ions
in the conductivity mechanism. The bridge character of the complexes also
contributed to their elec. conductivity
CC 76-2 (Electric Phenomena)

10/516884

IT 14325-24-7 39368-58-6 57756-65-7 57756-66-8 57756-67-9
57756-69-1 57756-70-4 57756-71-5 57756-73-7 58098-47-8

RL: PRP (Properties)
(elec. conductivity of)

IT 57756-73-7

RL: PRP (Properties)
(elec. conductivity of)

RN 57756-73-7 ZCAPLUS

CN Cobaltate(6-), aqua-μ-hydroxyhydroxybis[29H,31H-phthalocyanine-C,C,C,C-
tetrasulfonato(6-)-N29,N30,N31,N32]di-, sodium sulfate (1:8:1) (9CI) (CA
INDEX NAME)

CM 1

CRN 57756-72-6

CMF C64 H28 Co2 N16 O27 S8

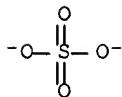
CCI CCS, IDS

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

CM 2

CRN 14808-79-8

CMF O4 S



=> d his full

(FILE 'HOME' ENTERED AT 07:55:03 ON 07 DEC 2007)

FILE 'REGISTRY' ENTERED AT 07:57:31 ON 07 DEC 2007

ACT WAR884RNS/A

L1 21 SEA ABB=ON PLU=ON (123833-60-3/BI OR 13450-90-3/BI OR
13478-18-7/BI OR 13930-88-6/BI OR 14154-42-8/BI OR 15746-68-6/B
I OR 168216-37-3/BI OR 19717-79-4/BI OR 26201-32-1/BI OR
634179-07-0/BI OR 634179-08-1/BI OR 634179-09-2/BI OR 634179-10
-5/BI OR 634179-11-6/BI OR 634179-46-7/BI OR 634179-47-8/BI OR
634179-48-9/BI OR 7446-70-0/BI OR 7550-45-0/BI OR 7718-98-1/BI
OR 91-15-6/BI)

ACT WAR884RNS/A

L*** DEL 21 SEA FILE=REGISTRY ABB=ON PLU=ON (123833-60-3/BI OR 13450-90-3

ACT WAR884HITRNS/A

L2 (21)SEA ABB=ON PLU=ON (123833-60-3/BI OR 13450-90-3/BI OR
13478-18-7/BI OR 13930-88-6/BI OR 14154-42-8/BI OR 15746-68-6/B
I OR 168216-37-3/BI OR 19717-79-4/BI OR 26201-32-1/BI OR
634179-07-0/BI OR 634179-08-1/BI OR 634179-09-2/BI OR 634179-10
-5/BI OR 634179-11-6/BI OR 634179-46-7/BI OR 634179-47-8/BI OR
634179-48-9/BI OR 7446-70-0/BI OR 7550-45-0/BI OR 7718-98-1/BI
OR 91-15-6/BI)

L3 7 SEA ABB=ON PLU=ON L2 AND NRS>1

ACT WAR884STR20L/A

L4 STR

L5 2661 SEA SSS FUL L4

ACT WAR884STR27L/A

L6 STR

L7 (2661)SEA SSS FUL L6

L8 STR

L9 227 SEA SUB=L7 SSS FUL L8

ACT WAR884STR40L/A

L10 STR

L11 (2661)SEA SSS FUL L10

L12 STR

L13 206 SEA SUB=L11 SSS FUL L12

FILE 'ZCAPLUS' ENTERED AT 08:04:54 ON 07 DEC 2007

L*** DEL 3080 S L!3

L14 157 SEA ABB=ON PLU=ON L13

FILE 'REGISTRY' ENTERED AT 08:43:31 ON 07 DEC 2007

L15 STRUCTURE UPLOADED

L16 6 SEA SUB=L5 SSS SAM L15

L17 58 SEA SUB=L5 SSS FUL L15

10/516884

SAVE TEMP WAR884STR15B/A L17

L18 FILE 'ZCAPLUS' ENTERED AT 08:45:14 ON 07 DEC 2007
50 SEA ABB=ON PLU=ON L17

FILE 'REGISTRY' ENTERED AT 08:45:34 ON 07 DEC 2007
D SCA L17

L19 6 SEA ABB=ON PLU=ON L17 AND ?SULFONYL?/CNS
D SCA

L20 52 SEA ABB=ON PLU=ON L17 NOT L19

L21 0 SEA ABB=ON PLU=ON L20 AND L3
D SCA L3

FILE 'ZCAPLUS' ENTERED AT 08:59:29 ON 07 DEC 2007

L22 50 SEA ABB=ON PLU=ON L20

FILE 'REGISTRY' ENTERED AT 09:00:52 ON 07 DEC 2007

L23 STRUCTURE UPLOADED

L24 STRUCTURE UPLOADED

L25 9 SEA SUB=L5 SSS SAM L24

L26 STRUCTURE UPLOADED

L27 STRUCTURE UPLOADED

L28 STRUCTURE UPLOADED

L29 9 SEA SUB=L5 SSS SAM L28

L30 111 SEA SUB=L5 SSS FUL L28

L31 0 SEA ABB=ON PLU=ON L3 AND L30

L32 STRUCTURE UPLOADED

L33 9 SEA SUB=L5 SSS SAM L32

L34 154 SEA SUB=L5 SSS FUL L32

L35 2 SEA ABB=ON PLU=ON L34 AND L3
D SCA
D SCA

L36 8 SEA ABB=ON PLU=ON L17 AND NC>1
D SCA

L37 1 SEA ABB=ON PLU=ON L36 AND HYDROXIDE/CNS

FILE 'ZCAPLUS' ENTERED AT 09:24:26 ON 07 DEC 2007

L38 1 SEA ABB=ON PLU=ON L37
D BIB

L*** DEL 0 S L34 AND NC>1

FILE 'REGISTRY' ENTERED AT 09:25:14 ON 07 DEC 2007

L39 39 SEA ABB=ON PLU=ON L34 AND NC>1
D SCA

FILE 'STNGUIDE' ENTERED AT 09:30:54 ON 07 DEC 2007

FILE 'REGISTRY' ENTERED AT 09:39:09 ON 07 DEC 2007

FILE 'STNGUIDE' ENTERED AT 09:42:34 ON 07 DEC 2007

FILE 'REGISTRY' ENTERED AT 09:47:20 ON 07 DEC 2007

L40 1 SEA ABB=ON PLU=ON L17 AND HYDROXIDE/CNS

L41 6 SEA ABB=ON PLU=ON L34 AND HYDROXIDE/CNS

L42 1 SEA ABB=ON PLU=ON L34 AND SULFATE/CNS
D SCA

L43 0 SEA ABB=ON PLU=ON L17 AND SULFATE/CNS

L44 154 SEA ABB=ON PLU=ON L17 OR L34

L45 1 SEA ABB=ON PLU=ON L44 AND CHLORIDE/CNS
D SCA

10/516884

L46 7 SEA ABB=ON PLU=ON (L40 OR L41 OR L42)
L47 2 SEA ABB=ON PLU=ON L46 AND L3
L48 5 SEA ABB=ON PLU=ON L46 NOT L47
D SCA

FILE 'ZCAPLUS' ENTERED AT 09:52:26 ON 07 DEC 2007

L49 4 SEA ABB=ON PLU=ON L48
D IBIB HITSTR L49 1-4
L50 5 SEA ABB=ON PLU=ON L46

FILE 'REGISTRY' ENTERED AT 09:55:05 ON 07 DEC 2007

SEL RN L46
SEL CRN L46
L51 8 SEA ABB=ON PLU=ON (14808-79-8/RN OR 57756-72-6/RN OR
753449-37-5/RN OR 763925-00-4/RN OR 788155-69-1/RN OR 878378-54
-2/RN OR 878378-55-3/RN OR 878378-56-4/RN)
D SCA
L52 1 SEA ABB=ON PLU=ON SULFATE/CN
L53 7 SEA ABB=ON PLU=ON L51 NOT L52

FILE 'ZCAPLUS' ENTERED AT 09:56:35 ON 07 DEC 2007

L54 0 SEA ABB=ON PLU=ON L53

FILE 'REGISTRY' ENTERED AT 09:57:38 ON 07 DEC 2007

L55 17925 SEA ABB=ON PLU=ON TETRAKIS/CNS (200W) TETRAKIS/CNS
L56 9 SEA ABB=ON PLU=ON L55 AND L34
D SCA
L57 1 SEA ABB=ON PLU=ON HYDROXIDE/CN
L58 1 SEA ABB=ON PLU=ON SULFATE/CN
L59 1 SEA ABB=ON PLU=ON CHLORIDE/CN
L60 0 SEA ABB=ON PLU=ON H S O/ELF
L61 30961 SEA ABB=ON PLU=ON H O S/ELF
L62 30964 SEA ABB=ON PLU=ON (L57 OR L58 OR L59 OR L60 OR L61)

FILE 'ZCAPLUS' ENTERED AT 10:01:32 ON 07 DEC 2007

L63 83 SEA ABB=ON PLU=ON L44
L64 50 SEA ABB=ON PLU=ON L17
L65 4 SEA ABB=ON PLU=ON L62 AND (L63 OR L64)
L66 4 SEA ABB=ON PLU=ON L65 NOT L50
D SCA
L67 1 SEA ABB=ON PLU=ON L66 AND SULFATE/OBI
L68 581403 SEA ABB=ON PLU=ON CHARGE/BI
L69 8 SEA ABB=ON PLU=ON (L63 OR L64) AND L68
D SCA
L70 362 SEA ABB=ON PLU=ON TAKAKI K?/AU
L71 929 SEA ABB=ON PLU=ON YAMASAKI Y?/AU
L72 7 SEA ABB=ON PLU=ON L70 AND L71
L73 3 SEA ABB=ON PLU=ON (L70 OR L71) AND (L38 OR L50 OR L67 OR
L69)

FILE 'REGISTRY' ENTERED AT 10:07:20 ON 07 DEC 2007

FILE 'ZCAPLUS' ENTERED AT 10:07:24 ON 07 DEC 2007

D STAT QUE L72
D STAT QUE L73
L74 7 SEA ABB=ON PLU=ON L72 OR L73
D IBIB ABS HITIND HITSTR L74 1-7

FILE 'REGISTRY' ENTERED AT 10:08:40 ON 07 DEC 2007

10/516884

FILE 'ZCAPLUS' ENTERED AT 10:08:44 ON 07 DEC 2007

D STAT QUE L38

D STAT QUE L50

D STAT QUE L67

D STAT QUE L69

L75 9 SEA ABB=ON PLU=ON (L38 OR L50 OR L67 OR L69) NOT (L72 OR L73)

D IBIB ABS HITIND HITSTR L75 1-9

FILE HOME

FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 6 DEC 2007 HIGHEST RN 957014-20-9

DICTIONARY FILE UPDATES: 6 DEC 2007 HIGHEST RN 957014-20-9

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FILE ZCAPLUS

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FILE STNGUIDE

FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Nov 30, 2007 (20071130/UP).

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